TENSORFLOW RIEMOPT: A LIBRARY FOR OPTIMIZATION ON Riemannian manifolds

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ABSTRACT

The adoption of neural networks and deep learning in non-Euclidean domains has been hindered until recently by the lack of scalable and efficient learning frameworks. Existing toolboxes in this space were mainly motivated by research and education use cases, whereas practical aspects, such as deploying and maintaining machine learning models, were often overlooked.

We attempt to bridge this gap by proposing TensorFlow RiemOpt, a Python library for optimization on Riemannian manifolds in TensorFlow. The library is designed with the aim for a seamless integration with the TensorFlow ecosystem, targeting not only research, but also streamlining production machine learning pipelines.

Keywords: large-scale machine learning, Riemannian optimization, neural networks

1 Introduction

Over the past years, there has been a surge of interest in machine learning in non-Euclidean domains. Representation learning in spaces of constant negative curvature, i.e. hyperbolic, has shown to outperform Euclidean embeddings significantly on data with latent hierarchical, taxonomic or entailment structures. Such data naturally arises in language modeling [29, 30, 38, 13], recommendation systems [10], image classification, and few-shot learning tasks [21], to name a few. Grassmannian manifolds find applications in computer vision to perform video-based face recognition and image set classification [19, 25]. The Lie groups of transformations SO(3) and SE(3) appear naturally when dealing with problems like pose estimation and skeleton-based action recognition [16, 18]. Stiefel manifolds are used for emotion recognition and action recognition from video data [8, 17]. The space of symmetric positive definite (SPD) matrices characterize data from diffusion tensor imaging [33], and functional magnetic resonance imaging [40]. Among those advances is a family of neural network methods, which are parameterized by weights constrained to a particular non-Euclidean space [29, 9, 18, 13, 10, 21].

Stochastic Gradient Descent (SGD) [35] algorithm has been used for the backpropagation learning in connectionist neural network models. The SGD is known to generate undesirable oscillations around optimal values of model parameters [34]. Using a momentum term [37] has been shown to improve the optimization convergence. More recently, adaptive learning rates [15, 22, 43] have been proposed, and are popular optimization algorithms used for iterative optimization while training neural networks.

These adaptations of the SGD methods have been studies extensively under the lenses of Riemannian geometry and translated to non-Euclidean settings [6, 36, 5, 20]. Riemannian stochastic optimization algorithms have been robustly integrated with many popular machine learning toolboxes. However, previous work in this space was mainly motivated by research use cases [42, 27, 28, 23]. Whereas practical aspects, such as deploying and maintaining machine learning models, were often overlooked.

We present TensorFlow RiemOpt, a Python library for optimization on Riemannian manifolds in TensorFlow [1], to help bridge the aforementioned gap. The library is designed with the aim for a seamless integration with the TensorFlow ecosystem, targeting not only research, but also end-to-end machine learning pipelines with the recently proposed TensorFlow Extended platform [4].
2 Riemannian optimization

In this section we provide a brief overview of Riemannian optimization with a focus on stochastic methods. We refer to \cite{8,39} for more rigorous theoretical treatment.

Optimization on Riemannian manifolds, or Riemannian optimization, is a class of methods for optimization of the form

\[ \min_{x \in \mathcal{M}} f(x) \]  

where \( f \) is an objective function, subject to constraints which are smooth, in the sense that the search space \( \mathcal{M} \) admits the structure of a differentiable manifold, equipped with a positive-definite inner product on the space of tangent vectors \( T_x \mathcal{M} \) at each point \( x \in \mathcal{M} \). Conceptually, the approach of Riemannian optimization translates the constrained optimization problem (1) into performing optimization in the Euclidean space \( \mathbb{R}^n \) and projecting the parameters back onto the search space \( \mathcal{M} \) after each iteration \( 2 \).

In particular, several first order stochastic optimization methods commonly used in the Euclidean domain, such as the SGD algorithm and related adaptive methods, have already been adapted to Riemannian settings.

The update equation of the (Euclidean) SGD for differentiable \( f \) takes the form

\[ x_{t+1} = x_t - \alpha \nabla f_t \]  

where \( \nabla f_t \) denotes the gradient of objective \( f \) evaluated at the minibatch taken at step \( t \), and \( \alpha > 0 \) is the learning rate. For a Riemannian manifold \( \mathcal{M} \), Riemannian SGD \( 6 \) performs the update

\[ x_{t+1} = \text{Exp}_{x_t}( - \alpha \pi_x \nabla f_t ) \]  

where \( \pi_x : \mathbb{R}^n \to T_x \mathcal{M} \) denotes the projection operator from the ambient Euclidean space on the tangent space \( T_x \mathcal{M} \). And \( \text{Exp}_x(u) : T_x \mathcal{M} \to \mathcal{M} \) is the exponential map operator, which moves a vector \( u \in T_x \mathcal{M} \) back to the manifold \( \mathcal{M} \) from the tangent space at \( x \).

In a neighborhood of \( x \), the exponential map identifies a point on the geodesic, thus guarantees decreasing the objective function. Intuitively, the exponential map enables to perform an update along the shortest path in the relevant direction in unit time, while remaining in the manifold. In practice, when \( \text{Exp}_x(u) \) is not known in closed-form or it is computationally expensive to evaluate, it is common to replace it by a retraction map \( R_x(u) \), which is a first-order approximation of the exponential.

Adaptive optimization techniques compute smoother estimates of the gradient vector using its first or second order moments. RMSProp \( 15 \) is an example of a gradient based optimization algorithm which does this by maintaining an exponentially moving average of the squared gradient, which is an estimate of the second raw moment of the gradient. The update equations for RMSProp can be expressed as follows

\[ m_{t+1} = \rho m_t + (1-\rho)(\nabla f_t \circ \nabla f_t) \]

\[ x_{t+1} = x_t - \alpha \frac{\nabla f_t}{\sqrt{m_{t+1} + \epsilon}} \]  

where \( \rho \) is a hyperparameter, \( \alpha \) is the learning rate, and \( \circ \) denotes the Hadamard product.

In the Euclidean settings, these estimates can be obtained by linearly combining previous moment vectors due to the inherent “flat” nature of the underlying space. However, since general Riemannian manifolds can be curved, it is not possible to simply add moment vectors at different points on the manifold, as the resulting vectors may not lie in the tangent spaces at either points.

Riemannian versions of adaptive SGD algorithms use the parallel transport to circumvent this issue \cite{36,5}. The parallel transport operator \( P_{x \to y}(v) \) : \( T_x \mathcal{M} \to T_y \mathcal{M} \) takes \( v \in T_x \mathcal{M} \) and outputs \( v' \in T_y \mathcal{M} \). Informally, \( v' \) is obtained by moving \( v \) in a “parallel” fashion along the geodesic curve connecting \( x \) and \( y \), where the intermediate vectors obtained through this process have constant norm and always belong to tangent spaces. Such transformation enables combining moment vectors computed at different points of the optimization trajectory.

Geometry-aware constrained RMSProp (cRMSProp) \cite{36} translates the Equation (4) to Riemannian settings as follows

\[ m_{t+1} = \rho P_{x_{t-1} \to x_t} m_t + (1-\rho) \pi_x (\nabla f_t \circ \nabla f_t) \]

\[ x_{t+1} = \text{Exp}_{x_t}( - \alpha \frac{\nabla f_t}{\sqrt{m_{t+1} + \epsilon}} ) \]  

2 Riemannian optimization

TensorFlow RiemOpt: a library for optimization on Riemannian manifolds

A PREPRINT
In practice, if $P_{x \rightarrow y}(v)$ is not known for a given Riemannian manifold or it is computationally expensive to evaluate, it is replaced by its first-order approximation $\tilde{P}_{x \rightarrow y}(v)$.

While many optimization problems are of the described form, technicalities of differential geometry and implementation of corresponding operators often pose a significant barrier for experimenting with these methods.

### 3 Design goals

Working out and implementing gradients is a laborious and error prone task, particularly when the objective function acts on higher rank tensors. TensorFlow RiemOpt builds upon the TensorFlow framework [1], and leverages its automatic differentiation capabilities for computing gradients of composite functions. The design of TensorFlow RiemOpt was informed by three main objectives:

1. **Interoperability with the TensorFlow ecosystem.** All components, including optimization algorithms and manifold-constrained variables, can be used as drop-in replacements with the native TensorFlow API. This ensures transparent integration with the rich ecosystem of tools and extensions in both research and production settings. Specifically, TensorFlow RiemOpt was tested to be compatible with the TensorFlow Extended platform in graph and eager execution modes.

2. **Computational efficiency.** TensorFlow RiemOpt aims for providing closed-form expressions for manifold operators. The library also implements numerical approximation as a fallback option, when such solutions are not available. TensorFlow RiemOpt solvers can perform updates on dense and sparse tensors efficiently.

3. **Robustness and numerical stability.** The library makes use of half-, single-, and double-precision arithmetic where appropriate.

### 4 Implementation overview

The package implements concepts in differential geometry, such as manifolds and Riemannian metrics with the associated exponential and logarithmic maps, geodesics, retractions, and transports. For manifolds, where closed-form expressions are not known, the library provides numerical approximations. The core module also exposes functions for assigning TensorFlow variables to manifold instances.

#### 4.1 Manifolds

The module `manifolds` is modeled after the Manopt [7] API, and provides implementations of the following manifolds:

- **Cholesky** – manifold of lower triangular matrices with positive diagonal elements [26]
- **Euclidian** – an unconstrained manifold with the Euclidean metric
- **Grassmannian** – manifold of $p$-dimensional linear subspaces of the $n$-dimensional space [12]
- **Hyperboloid** – manifold of $n$-dimensional hyperbolic space embedded in the $n+1$-dimensional Minkowski space
- **Poincare** – the Poincaré ball model of the hyperbolic space [29]
- **Product** – Cartesian product of manifolds [14]
- **SPDAffineInvariant** – manifold of symmetric positive definite (SPD) matrices endowed with the affine-invariant metric [33]
- **SPDLogCholesky** – SPD manifold with the Log-Cholesky metric [26]
- **SPDLogEuclidean** – SPD manifold with the Log-Euclidean metric [3]
- **SpecialOrthogonal** – manifold of rotation matrices
- **Sphere** – manifold of unit-normalized points
- **StiefelEuclidean** – manifold of orthonormal $p$-frames in the $n$-dimensional space endowed with the Euclidean metric
- **StiefelCanonical** – Stiefel manifold with the canonical metric [44]
- **StiefelCayley** – Stiefel manifold the retraction map via an iterative Cayley transform [24]
Each manifold is implemented as a Python class, which inherits the abstract base class `Manifold`. The minimal set of methods required for optimization includes:

- `inner(x, u, v)` – inner product (i.e., the Riemannian metric) between two tangent vectors $u$ and $v$ in the tangent space at $x$
- `proj(u, x)` – projection of a tangent vector $u$ in the ambient space on the tangent space at point $x$
- `retr(x, u)` – retraction $R_x(u)$ from point $x$ with given direction $u$. Retraction is a first-order approximation of the exponential map introduced in [6]
- `transp(x, y, v)` – vector transport $T_{x\to y}(v)$ of a tangent vector $v$ at point $x$ to the tangent space at point $y$. Vector transport is the first-order approximation of parallel transport

Selected manifolds also support exact computations for additional operators:

- `exp(x, u)` – exponential map $Exp_x(u)$ of a tangent vector $u$ at point $x$ to the manifold
- `log(x, y)` – logarithmic map $Log_x(y)$ of a point $y$ to the tangent space at $x$
- `ptransp(x, y, v)` – parallel transport $P_{x\to y}(v)$ of a vector $v$ from the tangent space at $x$ to the tangent space at $y$

All methods support broadcasting of tensors with different shapes to compatible shapes for arithmetic operations.

### 4.2 Optimizers

The module `optimizers` provides TensorFlow 2 API for optimization algorithms on Riemannian surfaces, including recently proposed adaptive methods:

- `RiemannianSGD` – stochastic Riemannian gradient descent [6]
- `ConstrainedRMSprop` – constrained RMSprop learning method [36]
- `RiemannianAdam` – Riemannian Adam and AMSGrad algorithms [5]

Algorithms are implemented to support dense and sparse updates, as well as serialization, which is crucial for compatibility with TensorFlow functions.

### 4.3 Layers

Finally, the module `layers` exemplify building blocks of neural networks, which can be used alongside with the native Keras [11] layers.

### 5 Usage

A simple illustrative example of using low-level API is depicted in Listing 1. There, TensorFlow RiemOpt closely follows the Manopt semantics and naming convention. Geometric meaning of those operations is visualized on Figure 1.

```python
import tensorflow_reimopt as reimopt

# Instantiate a manifold
S = reimopt.manifolds.Sphere()
x = S.projx(tf.constant([0.1, -0.1, 0.1]))
u = S.proju(x, tf.constant([1., 1., 1.]))
v = S.proju(x, tf.constant([-0.7, -1.4, 1.4]))

# Compute the exponential map and vector transports
y = S.exp(x, v)
u_ = S.transp(x, y, u)
v_ = S.transp(x, y, v)
```

Listing 1: Low-level API usage example
Constructing an optimization problem is demonstrated on Listing 2. Manifold-valued variables can be transparently passed to standard TensorFlow functions. And, conversely, native TensorFlow tensors are treated by TensorFlow RiemOpt algorithms as data in the Euclidean space.

```python
import tensorflow as tf
import tensorflow_reiopt as riemopt

# Number of training steps
STEPS = 10

# Instantiate a manifold
sphere = riemopt.manifolds.Sphere()

# Instantiate and assign a variable to the manifold
var = tf.Variable(sphere.random(shape=(N, 2)))
riemopt.variable.assign_to_manifold(var, sphere)

# Instantiate an optimizer algorithm
opt = riemopt.optimizers.RiemannianAdam(learning_rate=0.2)
pole = tf.constant([0., 1.])

# Compute the objective function and apply gradients
for _ in range(STEPS):
    with tf.GradientTape() as tape:
        loss = tf.linalg.norm(var - pole)
        grad = tape.gradient(loss, [var])
        opt.apply_gradients(zip(grad, [var]))
```

Listing 2: Optimization API usage example

6 Advanced Usage

The folder examples contains reference implementations of several neural network architectures with manifold-valued parameters. For example, the Rotation Mapping layer of the LieNet [18] with weights constrained to the SO(3) manifold is shown on Listing 3.
@tf.keras.utils.register_keras_serializable(name="RotMap")
class RotMap(tf.keras.layers.Layer):
    """ Rotation Mapping layer. """

    def build(self, input_shape):
        """ Create weights depending on the shape of the inputs. """

        Expected 'input_shape':
        '[batch_size, spatial_dim, temp_dim, num_rows, num_cols]', where
        'num_rows' = 3, 'num_cols' = 3, 'temp_dim' is the number of frames,
        and 'spatial_dim' is the number of edges.
        """
        input_shape = input_shape.as_list()
        so = SpecialOrthogonal()
        self.w = self.add_weight("w",
            shape=[input_shape[-4], input_shape[-2], input_shape[-1]],
            initializer=so.random,
        )
        assign_to_manifold(self.w, so)

    def call(self, inputs):
        return tf.einsum("sij ..., stjk ->...stik", self.w, inputs)

Listing 3: Layers API usage example

7 Related work

This section compares TensorFlow RiemOpt with related implementations on differential geometry and learning. While inspired by related work, the main difference of our library lies in the choice of the underlying framework and design objectives.

The library Geoopt [23] is the most closely related to TensorFlow RiemOpt. Geoopt is a research-oriented toolbox, which builds upon the PyTorch [31] library for tensor computation and GPU acceleration. Geoopt supports the Riemannian SGD, as well as adaptive optimization algorithms on Riemannian manifolds, and Markov chain Monte Carlo methods for sampling. However, PyTorch, being a research-first framework, lacks tooling for bringing machine learning pipelines to production, which limits Geoopt applicability in industrial settings.

McTorch [27] is a manifold optimization library for deep learning, that extends the PyTorch C++ code base to closely follow its architecture. McTorch supports Riemannian variants of stochastic optimization algorithms, and also implements a collection of neural network layers with manifold-constrained parameters. McTorch shares the same limitations as Geoopt due to its dependency on PyTorch.

Pymanopt [42] is a Python package that computes gradients and Hessian-vector products on Riemannian manifolds, and provides the following solvers: steepest descent, conjugate gradients, the Nelder-Mead algorithm, and the Riemannian trust regions. Pymanopt leverages on Theano [41] symbolic differentiation and on TensorFlow automatic differentiation for computing derivatives. Pymanopt is a great general-purpose tool for Riemannian optimization. However, it is not well-suited for neural network applications due to lack of support for SGD algorithms. It is also not intended for production use.

Lastly but not least, there is Geomstats [28] Python package for computations and statistics on nonlinear manifolds. Geomstats supports a broad list of manifolds such as hyperspheres, hyperbolic spaces, spaces of symmetric positive definite matrices and Lie groups of transformations. It also provides a modular library of differential geometry concepts, which includes the parallel transports, exponential and logarithmic maps, Levi-Civita connections, and Christoffel symbols. Geomstats focuses on research in differential geometry and education use cases, by providing low-level code that follows the Scikit-Learn [32] semantics. Geomstats examples also include a modified version of the Keras framework with support of the Riemannian SGD algorithm. However, it lacks engineering maintenance.

8 Conclusion

We propose TensorFlow RiemOpt, a library that combines optimization on Riemannian manifolds with automated differentiation capabilities of the TensorFlow framework. The library enables researchers to experiment with different
state of the art solvers for optimization problems in non-Euclidean domains, while also allowing practitioners to efficiently pursue large-scale machine learning. The benefits of TensorFlow RiemOpt are most noticeable when it comes to taking Riemannian machine learning models from research to production, where it unlocks advantages of TensorFlow tooling, such as continuous training and model validation.

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