

**Geoopt: Riemannian Optimization in PyTorch**

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**Abstract**

Geoopt is a research-oriented modular open-source package for Riemannian Optimization in PyTorch. The core of Geoopt is a standard Manifold interface which allows for the generic implementation of optimization algorithms [3]. Geoopt supports basic Riemannian SGD as well as adaptive optimization algorithms. Geoopt also provides several algorithms and arithmetic methods for supported manifolds, which allow composing geometry-aware neural network [4, 6, 9] layers that can be integrated with existing models.

```python
import geoopt
from geoopt.optim import (RiemannianAdam)
manifold = geoopt.Stiefel()
orth_mat = geoopt.Parameter(
    manifold.random(10, 10)
)
opt = RiemannianAdam([orth_mat])
```

Figure 1: Creation of a manifold valued parameter

Geoopt is built on top of PyTorch [11], a dynamic computation graph backend. This allows us to use all the capabilities of PyTorch for geometric deep learning, including autodifferentiation, GPU acceleration, and exporting models (e.g., ONNX [2]). Geoopt optimizers implement the interface of native PyTorch optimizers and can serve as a drop-in replacement during training. The only difference is how parameters are declared (see Figure 1). The created manifold parameters can be used transparently with PyTorch functions and its serialization utils. All native PyTorch tensors by Geoopt optimizers are treated as regular Euclidean parameters.

The work on the package is mostly motivated by experiments with hyperbolic embeddings and hyperbolic neural networks. We provide several models of hyperbolic space, including Poincaré model, Hyperboloid model, $k$-stereographic model which generalizes Hyperbolic, Euclidean, and Spherical geometries [1]. The Scaled wrapper scales parameterization of another manifold and allows learnable curvature in a different way [8]. ProductManifold constructs a product of existing manifolds and allows e.g., modeling mixed curvature. Geoopt also supports other basic manifolds like the Stiefel manifold of orthogonal matrices, BirkhoffPolytope for doubly stochastic ones, $n$-Sphere manifold, and the manifold formed by the intersection of a $n$-Sphere with a linear subspace.

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1https://github.com/geoopt/geoopt

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1 Design

Geoopt is not designed to solve all the use cases at once. Instead, we reduce concepts to just a few core methods required by optimizers. Geoopt aims to achieve a few goals:

1. Easy and intuitive implementation in existing models
2. Robust, numerically stable implementation of algorithms
3. Wide broadcasting support and product manifolds
4. Efficient optimization
5. Extensibility

We inherit from torch.Tensor and torch.nn.Parameter what gives compatibility across all the PyTorch library and leaves one and the only one way to use Geoopt within PyTorch code. This solves most API questions; if one has good knowledge of PyTorch, there should be no problem to use Geoopt since few levels of abstractions are required to learn. Optimizers can be used in the same way as PyTorch optimizers were used. geoopt.optim API was one of the priorities in the initial design draft. No other changes, but a different optimizer should be required for a user to perform Riemannian optimization. Such Optimizer API allows using 3rd party frameworks for training and experiment management since they usually assume an optimizer as a black box performing updates, and little control is given to a final user.

Robust implementation is another principle of Geoopt. PyTorch is considered to work with float32 precision, and memory constraints rarely allow us to use double precision. Therefore, if it is possible, algorithm implementation should be correct in single-precision too or at least not produce nan’s. In case it might not be accurate, there is a warning in documentation covering that case.

Broadcasting support is an assumed behavior in most of the PyTorch functionality. Without this support, we limit use-cases of the library and force users to write loops or rewrite code from scratch. That is why broadcasting is a valuable property of the library. Besides use-cases involving tensor manipulations, this also allows easy treatment of simple case product manifolds that broadcast along first dimensions. As for complex cases of product manifolds, geoopt.ProductManifold should solve the problem.

Optimization is a core idea of the library that should be done in the most efficient way possible. This usually includes optimizations in an update loop, merging operations of retraction, and parallel transport together. From a math point of view, this assumes factorization of the adaptive term. In product manifolds, the adaptive term is computed per manifold parameter, and product structure is exploited[3]. This is a part of Geoopt in the first place, and any possibility to make effective use of the adaptive term is implemented.

To extend Geoopt one should implement basic methods such as retraction or exponential map on the manifold, parallel or vector transport for tangent vectors, and make them properly broadcastable. The latter might be the hardest in implementation, and as maintainers, we are more than ready to help with it.

2 Advanced Features

The advanced usage of Geoopt covers Hyperbolic deep learning pioneered in recent years [5, 7, 10, 12, 13]. In Geoopt we provide a robust implementation for Poincare Ball model along with methods for performing supplementary math. Not only constant negative curvature is supported, but positive curvature stereographic model of a sphere is also a part of the unified implementation of Möbius arithmetics in projected spacetime domain. Users can find supplementary functions as methods of geoopt.Stereographic class. Varying curvature is allowed and claimed to be very robust to precision. Derivatives for curvature are supported for the whole domain and especially for zero curvature case.

Algorithms provided for the stereographic model are also broadcastable and can be used with semantics similar to PyTorch functions. Reduce and manifold dimensions can be specified by the user for convenience. We believe this should accelerate research in Hyperbolic deep learning. A robust
standalone implementation of gyrovector math takes time and effort from researches. Taking this burden to the library, everyone should benefit from the common good of open source.

Sometimes gradients may be sparse, and Riemannian optimization overhead makes sense. For such cases, we provide sparse versions of Riemannian Adam and SGD. They also may be found in the library.

3 Discussion

Some of the design choices may be found not perfect or extensible enough. No tool is to solve all the problems, and we will understand this. The library is written by enthusiast researches for enthusiast researches. During the work, there were refinements in API, design structure as newcomers found the library a bit complicated. This is true, goals stated in the proposal are hard to achieve without active communication and collaboration to combine math and engineering. The mission of Geoopt is to aggregate advances in Riemannian methods for deep learning and accelerate future findings.

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