

ManifoldsBase.jl – an interface for manifolds in Julia

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ABSTRACT

We present an overview about the interface of the Julia package `ManifoldsBase.jl` to define and work with manifolds in Julia. The package is a central component of the `JuliaManifolds` ecosystem and is used by nearly all other packages in the ecosystem and several packages in the Julia community.

We discuss the main design ideas of the interface and present an overview of the features and functions provided in `ManifoldsBase.jl` 2.0.

Keywords

Julia, Riemannian manifolds, Lie groups, differential geometry, numerical analysis, scientific computing

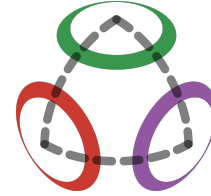
1. Introduction

In many scenarios one encounters data that does not lie in a Euclidean space. Informally phrased, for certain data, we are not allowed to just add or scale them. Examples are rotations, data on spheres, in hyperbolic spaces, symmetric positive definite matrices, like when working with covariance matrices, for example in processing diffusion tensor magnetic resonance images, or when the data is either bases of subspaces or subspaces themselves, i.e. data on the Stiefel, Grassmann or flag manifold. The data of interest for this paper still bear enough “structure”, i.e. they live on smooth manifolds.

In a prior paper about `Manifolds.jl` [3], a partial presentation of the interface of `ManifoldsBase.jl`¹ was given, when the interface was still in an early stage. A few fundamental design decisions have changed since then.

This paper presents the current state of the interface of `ManifoldsBase.jl` 2.0, since that state can be considered as having reached a very stable state. Its logo is shown in the Figure on the right.

The paper is organized as follows: in Section 2 we introduce the mathematical background and notation. In Section 4 we present the main design principles and structure of the interface. Section 3 presents the interface components in detail. In Section 6 we present an example of defining a new manifold, and Section 6 presents an overview of packages using `ManifoldsBase.jl`.



Logo of `ManifoldsBase.jl`.

2. Mathematical Background

This section introduces the mathematical background and notation used throughout this paper, for more details see, e.g. [7, 1, 5]. For differential geometry from a computational perspective see [6].

2.0.1 A topological manifold. A manifold \mathcal{M} is a topological space² that locally resembles Euclidean space \mathbb{R}^n , $n \in \mathbb{N}$. To make this more precise, for every point $p \in \mathcal{M}$, there exists a neighborhood $\mathcal{U} \subseteq \mathcal{M}$ and a homeomorphism $\varphi: \mathcal{U} \rightarrow \mathbb{R}^n$. The dimension of the manifold is defined as the dimension of the Euclidean space \mathbb{R}^n , which is the same for each point $p \in \mathcal{M}$. This can be interpreted as the number of degrees of freedom. The homeomorphism φ is called a *chart*, $\varphi(p)$ is called the *parameters* of the point p in the chart φ . A collection of charts $\varphi_i: \mathcal{U}_i \rightarrow \mathbb{R}^n$, $i \in \mathcal{I}$ for some index set \mathcal{I} , that cover the manifold $\mathcal{M} = \bigcup_i \mathcal{U}_i$ is called an *atlas*. If we can “smoothly change charts”, i.e. the transition maps $\varphi_j \circ \varphi_i^{-1}$ are smooth³, we say that the atlas \mathcal{A} is *smooth*. A manifold \mathcal{M} together with a smooth atlas is called a *smooth manifold*.

Informally, a smooth manifold allows us to compute derivatives on the manifold by “looking at it through a chart”. The smooth atlas then allows to argue, that this derivative is independent of the chosen chart.

As a guiding example, consider the n -dimensional sphere

$$\mathbb{S}^n = \{p \in \mathbb{R}^{n+1} \mid \|p\|_2 = 1\},$$

which is a smooth manifold of dimension n . A set of charts is for example the so-called *stereographic projections* onto the planes tangent to the sphere. Indeed, it is enough to consider the projections from the north and south pole to cover the sphere.

2.0.2 Tangent spaces. Consider any $p \in \mathcal{M}$ on a smooth manifold. In order to take (directional) derivatives at the point p , con-

¹Available at juliamanifolds.github.io/ManifoldsBase.jl/stable/, see also the Zenodo archive [2]

²We assume that the spaces we consider here are second countable and Hausdorff to exclude pathological examples.

³While one could consider different kinds of smoothness, C^1 , C^2 , ..., for simplicity one usually focuses on C^∞ .

sider the set of all smooth curves $c: (-\epsilon, \epsilon) \rightarrow \mathcal{M}$ with $c(0) = p$ that “run through p ”. To be precise, smoothness of the curve c means that for a chart φ with $p \in \mathcal{U}$, the map $c_\varphi(t) = \varphi(c(t))$ is a smooth in the classical sense as a map from $(-\epsilon, \epsilon)$ to \mathbb{R}^n . Since transitions of charts are smooth, this is independent of the choice of the actual chart. Hence we can now consider the derivative $\dot{c}_\varphi(0) \in \mathbb{R}^n$ of the curve in the chart φ_i . This can again be made independent of the chart and we obtain $\dot{c}(0)$.

In a single chart, any derivative $\dot{c}_\varphi(0)$ is equivalent to the first order to the curve $t \rightarrow \varphi^{-1}(\varphi(p) + bt)$ for some $b \in \mathbb{R}^n$. The vector b contains *coordinates* of the tangent vector in a basis induced by φ . Identifying each derivative $\dot{c}(0)$ with its coordinates b in a chart φ thus results in a one-to-one correspondence between curves through p and vectors in \mathbb{R}^n , formally this identification yields equivalence classes of curves. Overall we obtain the *tangent space* $T_p\mathcal{M}$ at $p \in \mathcal{M}$, which is a vector space of dimension n . Informally speaking, the tangent space contains all directions in which one can tangentially pass through the point p on the manifold \mathcal{M} . This is (again) independent of the choice of chart and we denote a tangent vector at p by $X \in T_p\mathcal{M}$. The disjoint union of all tangent spaces $T\mathcal{M} = \bigcup_{p \in \mathcal{M}} T_p\mathcal{M}$ is called the *tangent bundle*. As an example, on the sphere \mathbb{S}^n the tangent space at a point $p \in \mathbb{S}^n$ is given by

$$T_p\mathbb{S}^n = \{X \in \mathbb{R}^{n+1} \mid X^T p = 0\},$$

i.e. the set of all vectors in \mathbb{R}^{n+1} that are orthogonal to p . Visually, these are all vectors that are tangent to the sphere at the point p . On Euclidean space, the one chart $\varphi(p) = p$ is enough to cover the whole space and we obtain that all tangent spaces are isomorphic to \mathbb{R}^n itself.

The set of operations available on a smooth manifold is very limited, so in practice one has to extend it to be able to analyze some manifold-valued data. One of the most common ways is introducing inner product $\langle \cdot, \cdot \rangle_p: T_p\mathcal{M} \times T_p\mathcal{M} \rightarrow \mathbb{R}$ on each tangent space $T_p\mathcal{M}$. With two tangent vector fields $\mathcal{X}, \mathcal{Y}: \mathcal{M} \rightarrow T\mathcal{M}$, $\mathcal{X}(p), \mathcal{Y}(p) \in T_p\mathcal{M}$, we can consider the function $p \mapsto \langle \mathcal{X}(p), \mathcal{Y}(p) \rangle_p$. We say family of inner products $\langle \cdot, \cdot \rangle_p$ is *smoothly varying* (in p) if this map is a smooth map.

A *Riemannian manifold* is a smooth manifold \mathcal{M} together with a smoothly varying inner product on the tangent spaces $T_p\mathcal{M}$, called the *Riemannian metric*.

—geodesic, exp, log, parallel transport

—affine connection, there is a default for inner products.

3. The interface working with manifolds

3.1 Main types

The central type to represent a manifold is `AbstractManifold{ \mathbb{F} }` to represent a Riemannian manifold. The type parameter \mathbb{F} indicates, whether the representation of points and tangent vectors are arrays or data types over the reals \mathbb{R} , complex numbers \mathbb{C} or quaternions \mathbb{H} . A concrete manifold type should be a subtype of `AbstractManifold{ \mathbb{F} }` and contain all information about the manifold, most prominently its dimension. To build a possibly hierarchical structure of points or tangent vectors, the abstract types `AbstractManifoldPoint` and `AbstractTangentVector` exist⁴. These are, however not neces-

⁴the tangent vector type is more precisely a `AbstractFibreVector{TangentSpaceType}`, since other vector spaces can be modelled as well

sary to define or use the interface. For example the sphere can be used with plain `Vector{Float64}` as well. We recommend to use these as supertypes when defining new manifold point or tangent vector types, especially when these are mainly used to avoid type piracy.

3.2 General scheme of functions

Functions within `ManifoldsBase.jl` have a consistent order of arguments. The first argument should always be the manifold, followed by points and tangent vectors, and finally possibly positional arguments. When ever a function computes or returns a point, tangent vector, or array, both an allocating and an in-place version are available. The in-place version has an additional argument at the second position, i.e. directly following the manifold. For example generating a zero vector in the tangent space at a point p on a manifold \mathcal{M} is either `zero_vector(M, p)` or `zero_vector!(M, X, p)` to return the result in the pre-allocated vector X . By default, the allocating version should allocate a result and call the in-place version. This can be realised by using `allocate_result(M, f, args...)` for a function `f(M, args...)`. This allows to for example allocate the correct type of a tangent vector, when the arguments only contain the manifold and points. This is the case for example in the function `zero_vector(M, p)`.

3.3 Topological functions

Given a manifold \mathcal{M} , the following functions are defined to work with its topological structure. One can determine the dimension of the manifold with `manifold_dimension(M)`. A related function is `representation_size(M)`, that returns the array dimensions of a point or tangent vector in default representation, if this is applicable. If there is no default array representation, this function returns `nothing`. Points and tangent vectors can be represented in different ways. To distinguish these, one can pass a point type as positional second argument⁵. Whether a point p is a valid point on the manifold \mathcal{M} can be checked with `is_point(M, p)`. Similarly, whether a tangent vector X is a valid tangent vector in $T_p\mathcal{M}$ can be checked with `is_vector(M, p, X)`. By default the point p is checked as well, but with `check_base_point=false` this can be disabled. To check whether two points p and q or two tangent vectors X and Y are approximately equal, one can use `isapprox(M, p, q)` and `isapprox(M, p, X, Y)`, respectively. All three functions just return true or false by default, but one can also obtain more information in case of the function returning false by setting `error=:error`, `:warn`, or `:info`, specifying how to handle the error.

Furthermore the functions `copy(M, p)` and `copy(M, p, X)`, as well as `copyto!(M, q, p)` and `copyto!(M, Y, p, X)` create copies of or copy over values of one point to another.

We also extend the `rand` interface: `rand(M)` generates a random point, `rand(M; vector_at=p)` a random tangent vector. Both can be used with a random number generator as additional first argument. Random points and tangent vectors can also be generated in-place using `rand!(M, p)` and `rand!(M, X; vector_at=p)`.

—`get_embedding(M)`

—`embed(M, p) & embed(M, p, X)`

—`project(M, p) & project(M, p, X)` (mention `embed_project`.)

⁵**TODO: currently only concrete type.**

Table 1. : Retraction types available in ManifoldsBase.jl 2.0.

Retraction	comment/code
ApproximateRetraction	(internal)
EmbeddedRetraction{R}	use retraction R in the embedding
ExponentialRetraction	falls back to exp
PadeRetraction{m}	of order m
PolarRetraction	
ProductRetraction{R,S,...}	
ProjectionRetraction	falls back to project
QRRetraction	
SasakiRetraction	
SoftmaxRetraction	
StabilizedRetraction	

Table 2. : Inverse retraction types available in ManifoldsBase.jl 2.0.

Inverse retraction	comment/code
ApproximateInverseRetraction	
EmbeddedInverseRetraction{R}	use R in the embedding
InverseProductRetraction{R,S,...}	
LogarithmicInverseRetraction	falls back to log
PadeInverseRetraction	
PolarInverseRetraction	
ProjectionInverseRetraction	falls back to project
QRInverseRetraction	
SoftmaxInverseRetraction	

—zero_vector(M, p)
—retract(M, p, X, m)
—retract_fused(M, p, X, t, m) (in footnote?)
—Bases
—get_coordinates(M, p, X, b) &
get_vector(M, p, c, b)
—Charts & Atlases

3.4 Functions on manifolds with an affine connection

—exp(M, p, X)
—exp_fused(M, p, X, t) (in footnote?)
—geodesic(M, p, X, t)
—shortest_geodesic(M, p, q, t)
—injection_radius(M, p)
—log(M, p, q)
—inverse_retract(M, p, q, m)
—_is_flat(M)
—parallel_transport_to(M, p, X, p)
—parallel_transport_direction(M, p, X, d)
—riemannian_tensor(M, p, X, Y, Z)
—sectional_curvature(M, p, X, Y) (mention max/min)
—vector_transport_to(M, p, X, q, vtm)
—vector_transport_direction(M, p, X, d, vtm)

3.5 Functions on Riemannian manifolds

—inner(M, p, X, Y)

⁶This vector transport is a `AbstractLinearVectorTransportMethod`, i.e. it is linear in X .

Table 3. : Vector transport types available in ManifoldsBase.jl 2.0.

Vector transport	comment/code
DifferentiatedRetractionVectorTransport{R} ¹	induced by retraction R
EmbeddedVectorTransport{V}	use V in the embedding
ParallelTransport ⁶	uses <code>parallel_transport_to</code>
PoleLadderTransport ⁶	
ProjectionTransport ⁶	
ProductVectorTransport{V,W,...}	
ScaledVectorTransport	
SchildsLadderTransport ⁶	

—angle(M, p, X, Y)
—norm(M, p, X)
—distance(M, p, q)
—Weingarten(M, p, X, V)

4. The Interface to define new manifolds.

This section presents the main data structures and design principles of `ManifoldsBase.jl`.

4.1 Avoiding ambiguities with 3 layers of multiple dispatch.

Multiple dispatch is used in three separate layers to avoid ambiguities. The parameters of a function are groups into three parts: the manifold, the points and tangent vectors, and finally positional arguments. A concrete example would be the retraction `retract(M, p, X, m)`, that besides a manifold M , a point p and a tangent vector X at $p \in M$, has a positional m as the type of retraction, that has a reasonable default.

Layer I. On the first layer, only the manifold type should be used to dispatch the function. This allows to define functions for specific manifolds or generic manifold types. This layer should pass on to layer two. A user working on manifolds should usually only interact with functions defined on this layer.

Layer II. On the second layer, dispatching on certain positional arguments should be done. This allows to define functions that depend on specific positional arguments for all manifolds. Functions in this layer should be prefixed with an underscore `_` and should pass on to layer three. For our retraction example, this would be `_retract(M, p, X, ::ExponentialRetraction)` which would pass to the exponential map for any manifold with any point/tangent vector representation.

Layer III. On the third layer, dispatching on the point and tangent vector types should be done. This is usually also on concrete manifold types. Functions on this layer should usually have a postfix indicating the kind of positional arguments or be prefixed with two underscores. This layer would allocate a result and call the in-place version of the same function. A user implementing a new manifold would usually only have to implement the in-place functions on this layer. For a retraction example, consider the `ProjectionRetraction`, for which layer two would pass to a function `retract_project(M, p, X)`. This function would allocate the result Y and call `retract_project!(M, Y, p, X)`. This function defaults to calling `project!(M, Y, p, X)`, but also allows a user to implement a more efficient version, either for a specific manifold or for specific point or tangent vector types.

If there are no positional arguments, layer two and hence functions with the double underscore prefix or a suffix can be skipped.

4.2 A trait system to avoid code duplication.

Certain properties of a manifold can be accessed via traits⁷. This aims to avoid code duplication. A manifold using this trait system has to use the `AbstractDecoratorManifold{ℱ}` as supertype. These manifolds usually decorate the a manifold to add or modify certain properties. To access the internally stored manifold, use `base_manifold(M)`, which has an optional parameter `depth=-1` indicating how many decorators to “unwrap” with a default to remove all.

Then, on layer one, function arguments are prefixed with an argument of type `AbstractForwardingType`, which is used to “forward” the function call, e. g. to the embedding.

They can also be “marked” as `StopForwardingType` to indicate, that something is not passed, but needs to actually be implemented. For the example of embedded manifolds, the `EmbeddedForwardingType` is used to distinguish between different types of embeddings, e. g. isometric or submanifold type embeddings and whether the representation does change or not.

As a concrete example consider again the sphere \mathbb{S}^n as embedded submanifold of \mathbb{R}^{n+1} . Here, the function `is_point(M, p)` is implemented by forwarding to first check that `p` is a point on the embedding manifold \mathbb{R}^{n+1} and then check that $\|p\|_2 = 1$. We avoid implementing the test in the embedding. Similarly since the sphere is an `IsometricallyEmbeddedManifold`, also `inner(M, p, X, Y)` is forwarded to the embedding using the `SimpleForwardingType`, i.e. without any changes to the point or tangent vector representation.

Adding numerical validation. By default, functions from the interface in `ManifoldsBase.jl` assume, that their input consists of valid points and tangent vectors and does not verify input or output values. For debugging and numerical verification purposes, the package provides the `ValidationManifold` as a special manifold. It is implemented as a wrapper around any existing Riemannian manifold, `M2 = ValidationManifold(M)` and provides additional checks of correctness for both input parameters and output values of any function from the interface. That is, that type calls `is_point` and `is_vector` on all points and tangent vectors, respectively. While by default these checks do result in errors, this can be changed setting the `error=` keyword to either `:warn` or `:info`.

5. An example

5.1 Defining an own manifold

5.2 Adding a second metric to an existing manifold

5.3 Implementing a generic algorithm on a manifold

6. Where the interface is used

—`Manifolds.jl`
 —`Manopt.jl` [4]
 —`ManifoldDiff.jl`
 —`ManifoldDiffEq.jl`
 —`GeometricKalman.jl`

⁷This is sometimes referred to as Tim Holy’s Traits Trick (THTT) from the issue github.com/JuliaLang/julia#2345

—`ExponentialFamilyManifolds.jl` (Mykola) - and a second one he built on that?

—`ROME.jl` (?)

7. References

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