

A Series of Talks on Riemannian Optimization

Introduction and Some Basics

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① Introduction

- Riemannian optimization;
- Applications;
- Smooth optimization framework;
- Research foci of Riemannian optimization;

② Embedded Submanifold

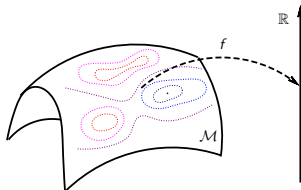
- Definition;
- Tangent space;
- Smooth maps;
- Vector fields and tangent bundle;
- Retraction;
- Riemannian Metric;
- A Riemannian steepest descent algorithm;

Riemannian Optimization

Problem: Given $f(x) : \mathcal{M} \rightarrow \mathbb{R}$, solve

$$\min_{x \in \mathcal{M}} f(x)$$

where \mathcal{M} is a Riemannian manifold.

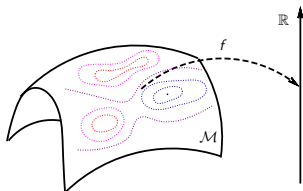


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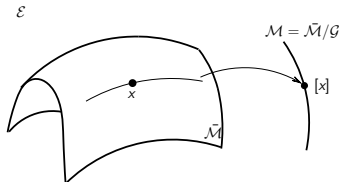


Two kinds of commonly-encountered manifolds

Embedded submanifold of a Euclidean space



Quotient manifold from an embedded submanifold

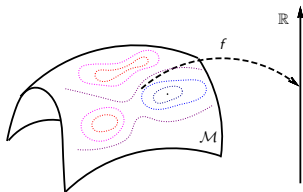


Riemannian Optimization

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Examples:

- Sphere: $\{x \in \mathbb{R}^n \mid \|x\| = 1\}$;
- Stiefel manifold:
 $\text{St}(p, n) = \{X \in \mathbb{R}^{n \times p} \mid X^T X = I_p\}$;
- Fixed rank:
 $\mathbb{R}_r^{m \times n} = \{X \in \mathbb{R}^{m \times n} : \text{rank}(X) = r\}$;
- etc;

Embedded submanifold of a Euclidean space

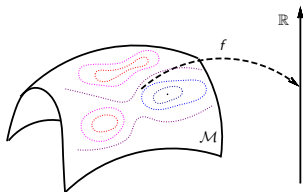


Riemannian Optimization

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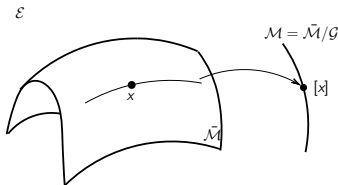
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Examples:

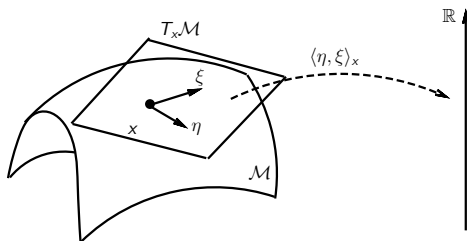
- Grassmann manifold:
the set of p dimensional linear spaces
in \mathbb{R}^n
 $\text{Gr}(p, n) = \text{St}(p, n) / \mathcal{O}_p$;
- Shape space;
- etc;

Quotient manifold from an embedded submanifold



Riemannian Optimization

Roughly, a Riemannian manifold \mathcal{M} is a smooth set with a smoothly-varying inner product on the tangent spaces.



Riemannian manifold = Manifold + Riemannian metric (inner products)

Applications

Embedded submanifold: Computation on SPD manifold

- SPD manifold:

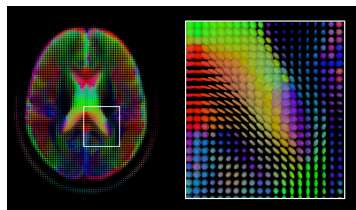
$$\mathcal{S}_{++}^n = \{X \in \mathbb{R}^{n \times n} : X = X^T, X \succ 0\};$$

- Applications of SPD matrices

- Diffusion tensors in medical imaging [CSV12, FJ07, RTM07]
- Describing images and video [LWM13, SFD02, ASF⁺05, TPM06, HWSC15]

- Motivation of averaging SPD matrices

- denoising / interpolation
- clustering / classification



Applications

Embedded submanifold: Computation on SPD manifold

One averaging SPD matrices method:

$$G(A_1, \dots, A_k) = \arg \min_{X \in \mathcal{S}_{++}^n} \frac{1}{2k} \sum_{i=1}^k \text{dist}^2(X, A_i),$$

where $\text{dist}(X, Y) = \|\log(X^{-1/2} Y X^{-1/2})\|_F$ is the distance under the Riemannian metric $\langle \eta_X, \xi_X \rangle = \text{trace}(\eta_X X^{-1} \xi_X X^{-1})$.

Applications

Embedded submanifold: Computation on SPD manifold

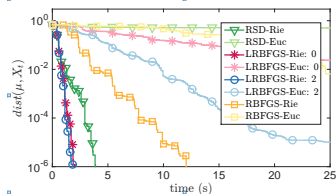
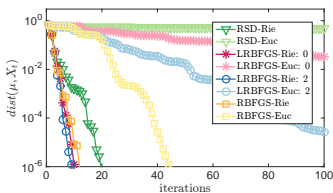
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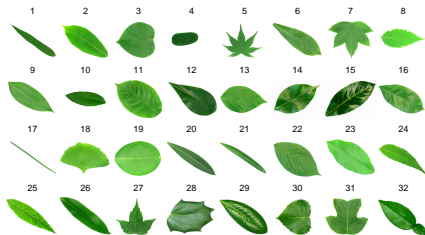
Why shall we use Riemannian optimization approach?

- $K = 30$, $n = 100$, and $1 \leq \kappa(A_i) \leq 10^5$.



Applications

Quotient manifold: Computation on shape space



- Classification
[LKS⁺12, HGSA15]
- Face recognition
[DBS⁺13]



Applications

Quotient manifold: Computation on shape space

- Elastic shape analysis invariants:
 - Rescaling
 - Translation
 - Rotation
 - Reparametrization
- The shape space is a quotient space

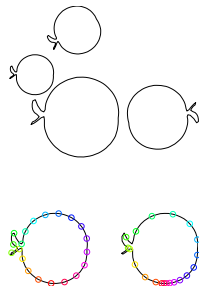
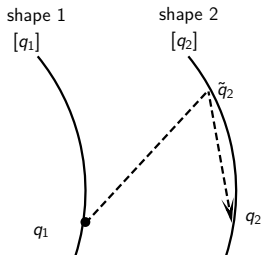


Figure: All are the same shape.

Applications

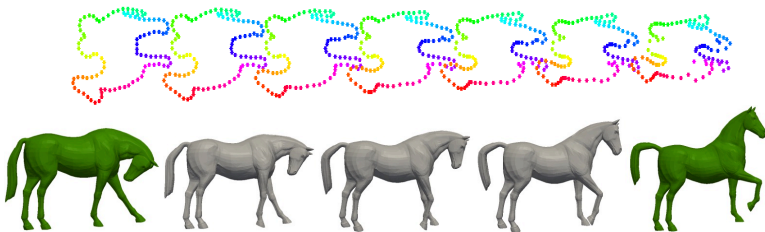
Quotient manifold: Computation on shape space Registration



- Optimization problem $\min_{q_2 \in [q_2]} \text{dist}(q_1, q_2)$ is defined on a Riemannian manifold

Applications

Quotient manifold: Computation on shape space Geodesic / Interpolation

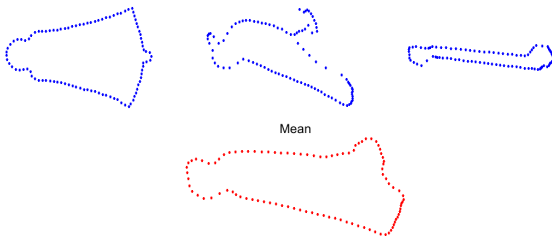


$$\min_{\alpha \in \mathcal{H}_{x,y}} \frac{1}{2} \int_0^1 \langle \dot{\alpha}(\tau), \dot{\alpha}(\tau) \rangle d\tau$$

- Computation of a geodesic between two shapes
- Interpolation in shape space

Applications

Quotient manifold: Computation on shape space Karcher mean

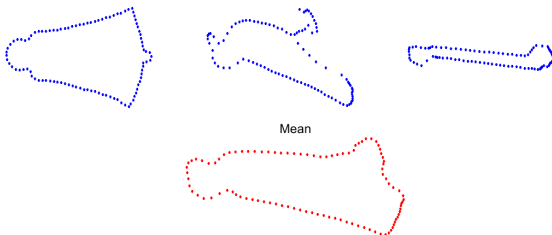


$$\min_{x \text{ is a shape}} \frac{1}{2k} \sum_{i=1}^k \text{dist}^2(X, S_i),$$

- Computation of Karcher mean of a population of shapes

Applications

Quotient manifold: Computation on shape space Karcher mean



$$\min_{x \text{ is a shape}} \frac{1}{2k} \sum_{i=1}^k \text{dist}^2(X, S_i),$$

- Computation of Karcher mean of a population of shapes

Riemannian optimization is used since these problems naturally involve a Riemannian manifold

Smooth Optimization Framework

Iterations on the Manifold

Consider the following generic update for an iterative Euclidean optimization algorithm:

$$x_{k+1} = x_k + \Delta x_k = x_k + \alpha_k s_k .$$

This iteration is implemented in numerous ways, e.g.:

- Steepest descent: $x_{k+1} = x_k - \alpha_k \nabla f(x_k)$
- Newton's method: $x_{k+1} = x_k - [\nabla^2 f(x_k)]^{-1} \nabla f(x_k)$
- Trust region method: Δx_k is set by optimizing a local model.

 $x_k + d_k$

Riemannian Manifolds Provide

- Riemannian concepts describing **directions** and **movement** on the manifold
- Riemannian analogues for **gradient** and **Hessian**

Smooth Optimization Framework

Riemannian gradient and Riemannian Hessian

Definition

The **Riemannian gradient** of f at x is the unique tangent vector in $T_x\mathcal{M}$ satisfying $\forall \eta \in T_x\mathcal{M}$, the directional derivative

$$Df(x)[\eta] = g(\text{grad}f(x), \eta)$$

and $\text{grad}f(x)$ is the direction of steepest ascent.

Definition

The **Riemannian Hessian** of f at x is a symmetric linear operator from $T_x\mathcal{M}$ to $T_x\mathcal{M}$ defined as

$$\text{Hess}f(x) : T_x\mathcal{M} \rightarrow T_x\mathcal{M} : \eta \rightarrow \nabla_\eta \text{grad}f,$$

where ∇ is the affine connection.

Smooth Optimization Framework

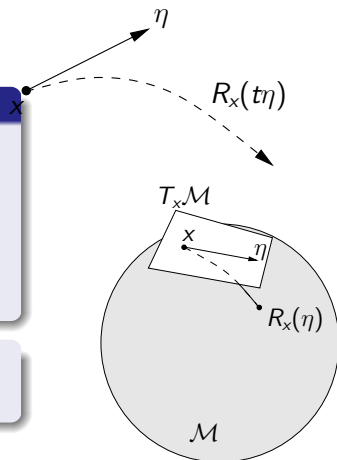
Retractions

Euclidean	Riemannian
$x_{k+1} = x_k + \alpha_k d_k$	$x_{k+1} = R_{x_k}(\alpha_k \eta_k)$

Definition

A **retraction** is a mapping R from $T\mathcal{M}$ to \mathcal{M} satisfying the following:

- R is continuously differentiable
- $R_x(0) = x$
- $DR_x(0)[\eta] = \eta$
- maps tangent vectors back to the manifold
- defines curves in a direction



Smooth Optimization Framework

Categories of Riemannian smooth optimization methods

Retraction-based: local information only

Line search-based: use local tangent vector and $R_x(t\eta)$ to define line

- Steepest decent
- Newton

Local model-based: series of flat space problems

- Riemannian trust region Newton (RTR)
- Riemannian adaptive cubic overestimation (RACO)

Smooth Optimization Framework

Categories of Riemannian smooth optimization methods

Retraction and transport-based: information from multiple tangent spaces

- Nonlinear conjugate gradient: multiple tangent vectors
- Quasi-Newton e.g. Riemannian BFGS: transport operators between tangent spaces

Additional element required for optimizing a cost function;

- formulas for combining information from multiple tangent spaces.

Smooth Optimization Framework

Categories of Riemannian smooth optimization methods

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Additional element required for optimizing a cost function;

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Vector Transport:

- Vector transport: Transport a tangent vector from one tangent space to another;
- $\mathcal{T}_{\eta_x} \xi_x$, denotes transport of ξ_x to tangent space of $R_x(\eta_x)$. R is a retraction associated with \mathcal{T} ;

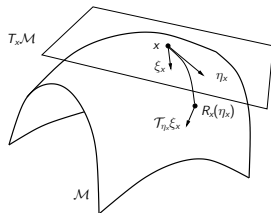


Figure: Vector transport.

Smooth Optimization Framework

Retraction/Transport-based Riemannian Optimization

Given a retraction and a vector transport, we can generalize classical unconstrained smooth optimization methods from Euclidean space to the Riemannian manifold.

Smooth Optimization Framework

Retraction/Transport-based Riemannian Optimization

Given a retraction and a vector transport, we can generalize classical unconstrained smooth optimization methods from Euclidean space to the Riemannian manifold.

Do the Riemannian versions of those methods work well?

Smooth Optimization Framework

Retraction/Transport-based Riemannian Optimization

Given a retraction and a vector transport, we can generalize classical unconstrained smooth optimization methods from Euclidean space to the Riemannian manifold.

Do the Riemannian versions of those methods work well?

No, generally

- Lose many theoretical results and important properties;
- Impose restrictions on retraction/vector transport;

Research Foci of Riemannian Optimization

- ① Manifold recognition, geometry structure analyses and computations;
 - ② Generalization Euclidean algorithms to the Riemannian setting;
 - ③ Algorithms specialization for applications;
 - ④ Library developments;
-

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- Manifold recognition
 - Riemannian metric
 - Retraction / Geodesic
 - Vector transport / Parallel translation

[EAS1998] A. Edelman, T. A. Arias, and S. T. Smith. The geometry of algorithms with orthogonality constraints. *SIAM Journal on Matrix Analysis and Applications*, 20(2):303–353, 1998

[CMV2017] T Carson, D. G. Mixon, and S. Villar. Manifold optimization for k-means clustering. In *2017 International Conference on Sampling Theory and Applications (SampTA)*, 73–77. IEEE, 2017

[SDN2021] G. Song, W. Ding, and M. K. Ng. Low rank pure quaternion approximation for pure quaternion matrices, *SIAM Journal on Matrix Analysis and Applications*, 42, pp. 58–82, 2021

[VAV2013] B. Vandereycken, P.-A. Absil, and S. Vandewalle. A Riemannian geometry with complete geodesics for the set of positive semidefinite matrices of fixed rank, *IMA Journal of Numerical Analysis*, 33.2, 481–514, 2013.

[Zim2017] R. Zimmermann. A matrix-algebraic algorithm for the Riemannian logarithm on the Stiefel manifold under the canonical metric. *SIAM Journal on Matrix Analysis and Applications*, 38.2, 322–342, 2017.

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- ① Manifold recognition, geometry structure analyses and computations;
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- Smooth unconstrained optimization algorithms
 - Nonsmooth unconstrained optimization algorithms
 - Constrained optimization algorithms

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Riemannian optimization mainly focuses on this topic.
Discuss later.

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- Computations on the SPD manifold;
- Computations on the shape space;
- Clustering and graph partitions;
- Beamforming in wireless communication;
- Blind source separation;
- etc

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- ① Manifold recognition, geometry structure analyses and computations;
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- Representation of a manifold and tangent spaces;
- Choose a Riemannian metric;
- Choose a retraction;
- Choose a vector transport;

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- Representation of a manifold and tangent spaces;
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Above factors may influence algorithms significantly.

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- Manopt (Matlab library) [Boumal, Mishra, Absil, Sepulchre(2014)]
- Pymanopt (Python version of Manopt) [Townsend, Koep, Weichwald (2016)]
- Manoptjl (Julia, nonsmooth methods) [Bergmann (2019)]
- ROPTLIB (C++ library, interfaces to Matlab and Julia)
[Huang, Absil, Gallivan, Hand (2018)]
- ManifoldOptim (R wrapper of ROPTLIB) [Martin, Raim, Huang, Adraghi (2018)]
- McTorch (Python, GPU acceleration)
[Meghawanshi, Jawanpuria, Kunchukuttan, Kasai, Mishra (2018)]
- CDOpt (Python, embedded submanifold in the form of $c(x) = 0$)
[Xiao, Hu, Liu, Toh (2022)]

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-

Provide theories to explain behaviors of existing algorithms for particular applications

- [MBDG2023]: IRKA is a Riemannian gradient descent method;
- [YHAG2020]: Richardson-like iteration for matrix geometric mean is a Riemannian gradient descent method;
- [BM2006]: The improved BFGS method is a Riemannian BFGS method using vector transport by parallelization;

[MBDG2023] P. Mlinaric, C. Beattie, Z. Drmac, and S. Gugercin. IRKA is a Riemannian Gradient Descent Method. [arxiv:2311.02031](https://arxiv.org/abs/2311.02031), 2023

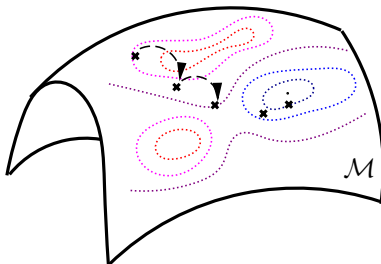
[YHAG2020] X. Yuan, W. Huang, P.-A. Absil, K. A. Gallivan. Computing the matrix geometric mean: Riemannian vs Euclidean conditioning, implementation techniques, and a Riemannian BFGS method, *Numerical Linear Algebra with Applications*, 27:5, 1-23, 2020

[BM2006] I. Brace and J. H. Manton. An improved BFGS-on-manifold algorithm for computing weighted low rank approximations. *Proceedings of 17th international Symposium on Mathematical Theory of Networks and Systems*, P.1735–1738, 2006

Comparison with Constrained Optimization

Not all Riemannian optimization problem can be formulated as constrained optimization problems, and vice versa.

- All iterates on the manifold
- Convergence properties of unconstrained optimization algorithms
- No need to consider Lagrange multipliers or penalty functions
- Exploit the structure of the constrained set



A Non-exhaustive Review

- Smooth unconstrained problems
 - Steepest descent: Smith 1994; Helmke-Moore 1994; Iannazzo-Porcelli 2019;
 - Conjugate gradient: Smith 1994; Gallivan-Absil 2010; Ring-Wirth 2012; Sato-Iwai 2015;
 - Quasi-Newton: Ring-Wirth 2012; Huang-Absil-Gallivan 2018; Huang-Gallivan 2022
 - Newton-CG: Absil-Baker-Gallivan 2007; Huang-Huang 2023
- Nonsmooth unconstrained problems
 - Proximal point method: Ferreira-Oliveira 2002;
 - Optimality conditions: Yang-Zhang-Song 2014;
 - Gradient sampling: Huang 2013; Hosseini and Uschmajew 2017;
 - ϵ -subgradient-based methods: Grohs-Hosseini 2015;
 - Proximal gradient methods: Huang-Wei 2022;
 - Proximal Newton method: Si-Absil-Huang-Jiang-Vary 2023;
- Constrained problems:
 - Augmented Lagrangian methods: Boumal-Liu 2019;
 - Sequential quadratic programming: Obara-Okuno-Takeda 2022;
 - Frank-Wolfe Methods: Weber-Sra 2023;

A Non-exhaustive Review

- Smooth unconstrained problems:
 - Stiefel manifold: Wen-Yin 2012; Jiang-Dai 2014; Xiao-Liu-Yuan 2020; Dai-Wang-Zhou 2020
 - Symplectic Stiefel manifold: Gao-Son-Absil-Stykel 2021
 - Symmetric positive definite manifold: Bini-Iannazzo 2013; Zhang 2017; Yuan-Huang-Absil-Gallivan 2020;
 - Fixed rank manifold: Wen-Yin-Zhang 2012; Mishra 2014; Sutti-Vandereycken 2021; Levin-Kileel-Boumal 2022
- Nonsmooth unconstrained problems:
 - Stiefel Manifold: Huang-Wei 2019; Chen-Ma-So-Zhang 2020; Xiao-Liu-Yuan 2020;
 - Fixed rank manifold: Cambier-Absil 2016;
 - Matrix manifolds: Zhou-Bao-Ding-Zhu 2022
 - Smooth equation constraints: Xiao-Liu-Toh 2023
- Constrained problems:
 - Stiefel + non-negativity: Jiang-Meng-Wen-Chen 2019;
 - Symmetric positive definite + zeros: Phan-Menickelly 2020;

Content

① Introduction

- Riemannian optimization;
- Applications;
- Smooth optimization framework;
- Research foci of Riemannian optimization;

② Embedded Submanifold

- Definition;
- Tangent space;
- Smooth maps;
- Vector fields and tangent bundle;
- Retraction;
- Riemannian Metric;
- A Riemannian steepest descent algorithm;

Main references

- *An Introduction to Optimization on Smooth Manifolds*,
Nicolas Boumal, Version of May 25 2020


A nice introduction for readers who do not have background
on Riemannian manifold

- *Optimization Algorithms on Matrix Manifolds*,
P.-A. Absil, R. Mahony, R. Sepulchre,
Princeton University Press, January 2008

More suitable for readers who are familiar with Riemannian manifold.

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Embedded submanifolds

Definitions

What is a smooth Riemannian manifold? (focus on Embedded submanifolds)

Embedded submanifolds

Definitions

What is a smooth Riemannian manifold? (focus on Embedded submanifolds)

- Embedding space: Euclidean space

-
- Linear spaces: \mathbb{R}^n , $\mathbb{R}^{n \times p}$, $\text{Sym}(n)$, \mathbb{C}^n , $\mathbb{R}^{n_1 \times n_2 \times n_3}$
 - Euclidean space: A linear space equipped with a Euclidean metric

Embedded submanifolds

Definitions

What is a smooth Riemannian manifold? (focus on Embedded submanifolds)

- Embedding space: Euclidean space
- Embedded submanifolds

Definition

Let \mathcal{M} be a subset of a linear space \mathcal{E} . We say \mathcal{M} is a embedded submanifold of \mathcal{E} if either of the following holds:

- 1 \mathcal{M} is an open subset of \mathcal{E} . Then we also call \mathcal{M} an open submanifold. if $\mathcal{M} = \mathcal{E}$, we also call it a linear manifold.
- 2 For a fixed integer $k \geq 1$ and for each $x \in \mathcal{M}$ there exists a neighborhood \mathcal{U} of x in \mathcal{E} and a smooth function $h : \mathcal{U} \rightarrow \mathbb{R}^k$ such that
 - If y is in \mathcal{U} , then $h(y) = 0$ if and only if $y \in \mathcal{M}$; and
 - $\text{rank} Dh(x) = k$.

Such a function h is called a local defining function for \mathcal{M} at x .

Embedded submanifolds

Definitions

What is a smooth Riemannian manifold? (focus on Embedded submanifolds)

- Embedding space: Euclidean space
- Embedded submanifolds

Example

Show that the unit sphere $\mathbb{S}^{n-1} = \{x \in \mathbb{R}^n : x^T x = 1\}$ is an embedded submanifold.

Embedded submanifolds

Definitions

What is a smooth Riemannian manifold? (focus on Embedded submanifolds)

- Embedding space: Euclidean space
- Embedded submanifolds

Example

Show that $\{(x_1, x_2) : x_1^2 - x_2^2 = 0\}$ is not an embedded submanifold.

Embedded submanifolds

Definitions

What is a smooth Riemannian manifold? (focus on Embedded submanifolds)

- Embedding space: Euclidean space
- Embedded submanifolds
- Topology

Definition

A subset \mathcal{U} of \mathcal{M} is open in \mathcal{M} if \mathcal{U} is the intersection of \mathcal{M} with an open subset of \mathcal{E} . This is called the subspace topology.

Embedded submanifolds

Definitions

What is a smooth Riemannian manifold? (focus on Embedded submanifolds)

- Embedding space: Euclidean space
- Embedded submanifolds
- Topology

Proposition

Let \mathcal{M} be an embedded submanifold of \mathcal{E} . Any open subset of \mathcal{M} is also an embedded (but not necessarily open) submanifold of \mathcal{E} , with same dimension and tangent spaces as \mathcal{M} .

Embedded submanifolds

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Example

Show that $\Delta_+^{n+1} = \{x \in \mathbb{R}^n : x_1 + \dots + x_n = 1 \text{ and } x_1, \dots, x_n > 0\}$ is an embedded submanifold.

Embedded submanifolds

Definitions

What is a smooth Riemannian manifold? (focus on Embedded submanifolds)

- Embedding space: Euclidean space
 - Embedded submanifolds
 - Topology
 - Tangent space
-

Definition

Let \mathcal{M} be a subset of \mathcal{E} . For all $x \in \mathcal{M}$, define:

$$T_x \mathcal{M} = \{c'(0) : c : I \rightarrow \mathcal{M} \text{ is smooth around } 0 \text{ and } c(0) = x\},$$

where I is an open subset of \mathbb{R} .

Embedded submanifolds

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-

Theorem

Let \mathcal{M} be an embedded submanifold of \mathcal{E} . Consider $x \in \mathcal{M}$ and the set $T_x\mathcal{M}$. If \mathcal{M} is an open submanifold, then $T_x\mathcal{M} = \mathcal{E}$. Otherwise, $T_x\mathcal{M} = \ker Dh(x)$ with h any local defining function at x .

Embedded submanifolds

Definitions

What is a smooth Riemannian manifold? (focus on Embedded submanifolds)

- Embedding space: Euclidean space
- Embedded submanifolds
- Topology
- Tangent space

Example

Derive an expression of $T_x\mathbb{S}^{n-1}$, where \mathbb{S}^{n-1} is the unit sphere.

Embedded submanifolds

Smooth maps

Smooth maps on smooth manifolds

Embedded submanifolds

Smooth maps

Smooth maps on smooth manifolds

- Definitions

Definition

Let \mathcal{M} and \mathcal{M}' be embedded submanifolds of \mathcal{E} and \mathcal{E}' . A map $F: \mathcal{M} \rightarrow \mathcal{M}'$ is smooth if and only if it admits a smooth extension $\bar{F}: \mathcal{U} \rightarrow \mathcal{E}'$ in a neighborhood \mathcal{U} of \mathcal{M} in \mathcal{E} , so that $F(x) = \bar{F}(x)$ for all $x \in \mathcal{M}$, that is, \bar{F} is the restriction of \bar{F} to \mathcal{M} : $F = \bar{F}|_{\mathcal{M}}$

Embedded submanifolds

Smooth maps

Smooth maps on smooth manifolds

- Definitions
-

Embedded submanifolds

Smooth maps

Smooth maps on smooth manifolds

- Definitions

Example

- Given a smooth extension of the function $f: \mathbb{S}^{n-1} \rightarrow \mathbb{R} : x \mapsto x^T A x$ on the unique sphere.
- Given an example of an embedded submanifold \mathcal{M} and a smooth function $f: \mathcal{M} \rightarrow \mathbb{R}$ for which there does not exist a smooth extension $\bar{f}: \mathcal{E} \rightarrow \mathbb{R}$ smooth on all of \mathcal{E} .

Embedded submanifolds

Smooth maps

Smooth maps on smooth manifolds

- Definitions
- Differential

Definition

The differential of $F: \mathcal{M} \rightarrow \mathcal{M}'$ at x is a linear operator $DF(x): T_x\mathcal{M} \rightarrow T_{F(x)}\mathcal{M}'$ defined by:

$$DF(x)[v] = \left. \frac{d}{dt} F(c(t)) \right|_{t=0},$$

where c is a smooth curve on \mathcal{M} passing through x at $t = 0$ with velocity v .

Embedded submanifolds

Smooth maps

Smooth maps on smooth manifolds

- Definitions
- Differential

Proposition

Let \bar{F} be a smooth extension of $F: \mathcal{M} \rightarrow \mathcal{M}'$. Therefore, $DF(x) = D\bar{F}(x)|_{T_x\mathcal{M}}$.

Embedded submanifolds

Smooth maps

Smooth maps on smooth manifolds

- Definitions
- Differential

Proposition

Let \bar{F} be a smooth extension of $F: \mathcal{M} \rightarrow \mathcal{M}'$. Therefore, $DF(x) = D\bar{F}(x)|_{T_x\mathcal{M}}$.

- $DF(x)$ is linear since $D\bar{F}(x)$ is linear.
- The definition of $DF(x)$ is independent of c with $c(0) = x$ and $c'(0) = v$.

Embedded submanifolds

Smooth maps

Smooth maps on smooth manifolds

- Definitions
- Differential

Example

Let $f: \mathbb{S}^{n-1} \rightarrow \mathbb{R} : x \mapsto x^T A x$, where $A = A^T$. Compute $Df(x)[v]$ for $v \in T_x \mathbb{S}^{n-1}$.

Embedded submanifolds

Smooth maps

Smooth maps on smooth manifolds

- Definitions
- Differential
- Properties of differentials

Example

Let $f: \mathcal{M} \rightarrow \mathbb{R}$, $F: \mathcal{M} \rightarrow \mathcal{M}'$ and $G: \mathcal{M}' \rightarrow \mathcal{M}''$ be smooth, where \mathcal{M} , \mathcal{M}' , and \mathcal{M}'' are embedded submanifolds of \mathcal{E} , \mathcal{E}' and \mathcal{E}'' respectively. Then

- Show that $fF: x \rightarrow f(x)F(x)$ is smooth from \mathcal{M} to \mathcal{E}' and we have product rule:

$$D(fF)(x)[v] = F(x)Df(x)[v] + f(x)DF(x)[v].$$

- Show that $D(G \circ F)(x)[v] = DG(F(x))[DF(x)[v]]$.

Embedded submanifolds

Tangent bundle and vector fields

Tangent bundle and vector fields

Embedded submanifolds

Tangent bundle and vector fields

Tangent bundle and vector fields

- Tangent bundle: Definition

Definition

The tangent bundle of a manifold \mathcal{M} is the disjoint union of the tangent spaces of \mathcal{M} :

$$T\mathcal{M} = \{(x, v) : x \in \mathcal{M} \text{ and } v \in T_x\mathcal{M}\}.$$

Note that the first component x is used for the notion of “disjoint” union when \mathcal{M} is an embedded submanifold. In the abstract definition of the tangent bundle, tangent spaces are disjoint by definition. It follows that $T\mathcal{M} = \cup_{x \in \mathcal{M}} T_x\mathcal{M}$.

Embedded submanifolds

Tangent bundle and vector fields

Tangent bundle and vector fields

- Tangent bundle: Definition

Theorem

If \mathcal{M} is an embedded submanifold of \mathcal{E} , the tangent bundle $T\mathcal{M}$ is an embedded submanifold of $\mathcal{E} \times \mathcal{E}$ of dimension $2\dim(\mathcal{M})$.

Embedded submanifolds

Tangent bundle and vector fields

Tangent bundle and vector fields

- Tangent bundle: Definition
 - Vector fields: Definition
-

Definition

A vector field on a manifold \mathcal{M} is a map $V: \mathcal{M} \rightarrow T\mathcal{M}$ such that $V(x)$ is in $T_x\mathcal{M}$ for all $x \in \mathcal{M}$. If V is a smooth map, we say it is a smooth vector field. The set of smooth vector fields is denoted by $\mathfrak{X}(\mathcal{M})$.

Embedded submanifolds

Tangent bundle and vector fields

Tangent bundle and vector fields

- Tangent bundle: Definition
 - Vector fields: Definition
-

Proposition

For \mathcal{M} an embedded submanifold of \mathcal{E} , a vector field V on \mathcal{M} is smooth if and only if there exists a smooth vector field \bar{V} on $\mathcal{U} \subseteq \mathcal{E}$ (a neighborhood of \mathcal{M}) such that $V = \bar{V}|_{\mathcal{M}}$.

Embedded submanifolds

Tangent bundle and vector fields

Tangent bundle and vector fields

- Tangent bundle: Definition
- Vector fields: Definition

Example

Give a smooth vector field on \mathbb{S}^{n-1} , where \mathbb{S}^{n-1} is the unit sphere.

Embedded submanifolds

Retraction

Retraction

Embedded submanifolds

Retraction

Retraction

- Definition

A retraction on \mathcal{M} is a smooth map $R: T\mathcal{M} \rightarrow \mathcal{M}$ with the following properties. For each $x \in \mathcal{M}$, let $R_x: T_x\mathcal{M} \rightarrow \mathcal{M}$ be the restriction of R at x , so that $R_x(v) = R(x, v)$. Then

- ① $R_x(0) = x$, and
- ② $DR_x(0): T_x\mathcal{M} \rightarrow T_x\mathcal{M}$ is the identity map: $DR_x(0)[v] = v$.

Equivalently, each curve $c(t) = R_x(tv)$ satisfies $c(0) = x$ and $c'(0) = v$.

Embedded submanifolds

Retraction

Retraction

- Definition

Example

Show that below two maps are retractions on \mathbb{S}^{n-1}

- $R_x(v) = \frac{x+v}{\|x+v\|}$, and
- $R_x(v) = \cos(\|v\|)x + \sin(\|v\|)\frac{v}{\|v\|}$,

where $v \in T_x\mathbb{S}^{n-1}$.

Embedded submanifolds

Retraction

Retraction

- Definition
- Recognition

Let \mathcal{M} be an embedded manifold of a vector space \mathcal{E} and let \mathcal{N} be an abstract manifold such that $\dim(\mathcal{M}) + \dim(\mathcal{N}) = \dim(\mathcal{E})$. Assume that there is a diffeomorphism $\phi : \mathcal{M} \times \mathcal{N} \rightarrow \mathcal{E}_* : (F, G) \mapsto \phi(F, G)$, where \mathcal{E}_* is an open subset of \mathcal{E} , with a neural element I in \mathcal{N} satisfying $\phi(F, I) = F, \forall F \in \mathcal{M}$.

Theorem [AMS08, Proposition 4.1.2]

The mapping

$$R_X(\xi) = \pi_1(\phi^{-1}(X + \xi))$$

defines a retraction \mathcal{M} , where $\pi_1 : \mathcal{M} \times \mathcal{N} \rightarrow \mathcal{M} : (F, G) \mapsto F$ is the projection onto the first component.

Embedded submanifolds

Retraction

Retraction

- Definition
- Recognition
- Construction

-
- Exponential mapping: $R_x(v) = \gamma(1)$, where $\gamma(t)$ is the geodesic such that $\gamma(0) = x$ and $\gamma'(0) = v$.
 - Retraction by projection: $R_x(v) = \arg \min_{y \in \mathcal{M}} \|x + v - y\|$
 - Orthographic retraction: $R_x(v) = x + v + u$, where $u \in T_x^\perp \mathcal{M}$.

See [AM12].

Embedded submanifolds

Riemannian metric

Riemannian metric

Embedded submanifolds

Riemannian metric

Riemannian metric

- Definition

Definition

An inner product on $T_x\mathcal{M}$ is a bilinear, symmetric, positive definite function $\langle \cdot, \cdot \rangle : T_x\mathcal{M} \times T_x\mathcal{M} \rightarrow \mathbb{R}$. It induces a norm for tangent vectors: $\|u\|_x = \sqrt{\langle u, u \rangle}$. A metric on \mathcal{M} is a choice of inner product $\langle \cdot, \cdot \rangle$ for each $x \in \mathcal{M}$.

Embedded submanifolds

Riemannian metric

Riemannian metric

- Definition

Definition

An inner product on $T_x\mathcal{M}$ is a bilinear, symmetric, positive definite function $\langle \cdot, \cdot \rangle : T_x\mathcal{M} \times T_x\mathcal{M} \rightarrow \mathbb{R}$. It induces a norm for tangent vectors: $\|u\|_x = \sqrt{\langle u, u \rangle}$. A metric on \mathcal{M} is a choice of inner product $\langle \cdot, \cdot \rangle$ for each $x \in \mathcal{M}$.

Definition

A metric $\langle \cdot, \cdot \rangle$ on \mathcal{M} is a Riemannian metric if it varies smoothly with x in the sense that if V, W are two smooth vector fields on \mathcal{M} then the function $x \mapsto \langle V(x), W(x) \rangle$ is smooth from \mathcal{M} to \mathbb{R} .

Embedded submanifolds

Riemannian metric

Riemannian metric

- Definition
- Riemannian manifold, Riemannian submanifold

Definition

A manifold with a Riemannian metric is a Riemannian manifold.

Embedded submanifolds

Riemannian metric

Riemannian metric

- Definition
- Riemannian manifold, Riemannian submanifold

Proposition

Let \mathcal{M} be an embedded submanifold of \mathcal{E} , and let $\langle \cdot, \cdot \rangle$ be the Euclidean metric on \mathcal{E} . Then, the metric on \mathcal{M} defined at each x by restriction, $\langle u, v \rangle = \langle u, v \rangle$ for $u, v \in T_x \mathcal{M}$ is a Riemannian metric.

Embedded submanifolds

Riemannian metric

Riemannian metric

- Definition
- Riemannian manifold, Riemannian submanifold

Proposition

Let \mathcal{M} be an embedded submanifold of \mathcal{E} , and let $\langle \cdot, \cdot \rangle$ be the Euclidean metric on \mathcal{E} . Then, the metric on \mathcal{M} defined at each x by restriction, $\langle u, v \rangle = \langle u, v \rangle$ for $u, v \in T_x \mathcal{M}$ is a Riemannian metric.

Definition

Let \mathcal{M} be an embedded submanifold of a Euclidean space \mathcal{E} . Equipped with the Riemannian metric obtained by restriction of the metric of \mathcal{E} , we call \mathcal{M} a Riemannian submanifold of \mathcal{E} .

Embedded submanifolds

Riemannian metric

Riemannian metric

- Definition
- Riemannian manifold, Riemannian submanifold
- Riemannian gradient

Definition

Let $f: \mathcal{M} \rightarrow \mathbb{R}$ be a smooth function on a Riemannian manifold \mathcal{M} . The Riemannian gradient of f is the vector field $\text{grad} f$ on \mathcal{M} uniquely defined by these identities:

$$\forall (x, v) \in T\mathcal{M}, Df(x)[v] = \langle v, \text{grad} f(x) \rangle,$$

where $\langle \cdot, \cdot \rangle$ is the Riemannian metric.

Embedded submanifolds

Riemannian metric

Riemannian metric

- Definition
 - Riemannian manifold, Riemannian submanifold
 - Riemannian gradient
-

Proposition

Let \mathcal{M} be a Riemannian submanifold of \mathcal{E} endowed with the Euclidean metric $\langle \cdot, \cdot \rangle$ and let $f: \mathcal{M} \rightarrow \mathbb{R}$ be a smooth function. The Riemannian gradient of f is given by

$$\operatorname{grad} f(x) = \operatorname{Proj}_x(\operatorname{grad} \bar{f}(x)),$$

where \bar{f} is a smooth extension of f to a neighborhood of \mathcal{M} in \mathcal{E} , and Proj_x denotes the orthogonal projection to $T_x\mathcal{M}$.

Embedded submanifolds

Riemannian metric

Riemannian metric

- Definition
 - Riemannian manifold, Riemannian submanifold
 - Riemannian gradient
-

Example

Derive the Riemannian gradient of $f: \mathbb{S}^{n-1} \rightarrow \mathbb{R} : x \mapsto x^T A x$, where the Riemannian metric is the Euclidean metric and $A = A^T$.

Embedded submanifolds

Riemannian metric

Riemannian metric

- Definition
 - Riemannian manifold, Riemannian submanifold
 - Riemannian gradient
-

Example

Show that the Riemannian gradient is unique by its definition.

Embedded submanifolds

Riemannian metric

Riemannian metric

- Definition
- Riemannian manifold, Riemannian submanifold
- Riemannian gradient

Example

Consider the relative interior of the simplex,

$$\mathcal{M} = \Delta_+^{n-1} = \{x \in \mathbb{R}^n : x_1, \dots, x_n > 0 \text{ and } x_1 + \dots + x_n = 1\},$$

as an embedded submanifold of \mathbb{R}^n . Its tangent spaces are given by

$$T_x \mathcal{M} = \{v \in \mathbb{R}^n : v_1 + \dots + v_n = 0\}.$$

Show that $\langle u, v \rangle = \sum_{i=1}^n \frac{u_i v_i}{x_i}$ defines a Riemannian metric on \mathcal{M} . Then, considering a smooth function $f: \mathcal{M} \rightarrow \mathbb{R}$ and a smooth extension \bar{f} on a neighborhood of \mathcal{M} in \mathbb{R}^n (equipped with the Euclidean metric), give an expression for $\text{grad} f(x)$ in terms of $\text{grad} \bar{f}(x)$.

Embedded submanifolds

A Riemannian steepest descent algorithm

A Riemannian steepest descent algorithm

Embedded submanifolds

A Riemannian steepest descent algorithm

A Riemannian steepest descent algorithm

- A Riemannian gradient descent algorithm

A representative Riemannian steepest descent algorithm:

- 1: Given: Initial step size $\sigma > 0$; Shrinking parameter $\rho \in (0, 1)$; $c \in (0, 1)$; initial iterate $x_0 \in \mathcal{M}$;
- 2: **for** $k = 0, 1, 2, \dots$ **do**
- 3: Find the largest $\alpha \in \{\sigma, \sigma\rho, \sigma\rho^2, \dots, \}$ such that

$$f(R_{x_k}(-\alpha \operatorname{grad} f(x_k))) \leq f(x_k) - c\alpha \|\operatorname{grad} f(x_k)\|_{x_k}^2$$

- 4: Set $x_{k+1} = R_{x_k}(-\alpha \operatorname{grad} f(x_k))$.
- 5: **end for**

Embedded submanifolds

A Riemannian steepest descent algorithm

A Riemannian steepest descent algorithm

- A Riemannian gradient descent algorithm
- First-order optimality conditions

Theorem

Let $f: \mathcal{M} \rightarrow \mathbb{R}$ be a smooth function on a Riemannian manifold. If x is a local minimizer of f , then $\text{grad} f(x) = 0$.

Embedded submanifolds

A Riemannian steepest descent algorithm

A Riemannian steepest descent algorithm

- A Riemannian gradient descent algorithm
- First-order optimality conditions

Theorem

Let $f: \mathcal{M} \rightarrow \mathbb{R}$ be a smooth function on a Riemannian manifold. If x is a local minimizer of f , then $\text{grad}f(x) = 0$.

Definition

Given a smooth function f on a Riemannian manifold \mathcal{M} , we call $x \in \mathcal{M}$ a critical point or a stationary point of f if $\text{grad}f(x) = 0$.

Embedded submanifolds

A Riemannian steepest descent algorithm

A Riemannian steepest descent algorithm

- A Riemannian gradient descent algorithm
- First-order optimality conditions
- Convergence

Assumption

- 1 *There exists $f_{\text{low}} \in \mathbb{R}$ such that $f(x) \geq f_{\text{low}}$ for all $x \in \mathcal{M}$.*
- 2 *For a given subset S of the tangent bundle $\mathcal{T}\mathcal{M}$, there exists a constant $L > 0$ such that, for all $(x, s) \in S$,*

$$f(R_x(s)) \leq f(x) + \langle \text{grad} f(x), s \rangle + \frac{L}{2} \|s\|^2.$$

Embedded submanifolds

A Riemannian steepest descent algorithm

A Riemannian steepest descent algorithm

- A Riemannian gradient descent algorithm
- First-order optimality conditions
- Convergence

Theorem

Let f be a smooth function satisfying the assumptions. Let $\{(x_i, s_i)\}_{i=0}^{\infty}$ be the pairs generated by the algorithm. If these pairs are in S defined in the assumption, then

$$\lim_{k \rightarrow \infty} \|\text{grad} f(x_k)\| = 0.$$

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