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Mini-Workshop: Approximation of Manifold-Valued Functions

Organized by
Nir Sharon, Tel Aviv
Holger Wendland, Bayreuth
Ralf Zimmermann, Odense

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Abstract. The approximation of unknown functions from scattered, possibly high-dimensional data is central to many scientific applications. Advances in data acquisition have driven the need for flexible nonlinear models, including manifold-valued functions. Approximating and learning such functions differs fundamentally from classical linear methods and requires tools from numerical analysis, linear algebra, and differential geometry. This interdisciplinary framework has applications ranging from data science and machine learning to numerical PDEs and quantum chemistry. This mini-workshop brings together researchers developing constructive approximation methods for manifold-valued functions, their theory, and applications.

Mathematics Subject Classification (2020): 65-00, 53-00.

Introduction by the Organizers

The mini-workshop Approximation of Manifold-Valued Functions brought together researchers from numerical analysis, approximation theory, differential geometry, and related areas to discuss recent advances and emerging challenges in the approximation, analysis, and computation of functions taking values in nonlinear spaces. With manifold-valued data becoming increasingly prevalent in modern applications, from computer vision and machine learning to model reduction, scientific computing, and physics, the need for mathematically sound and computationally efficient approximation techniques has grown substantially. The workshop aimed to foster interactions across disciplinary boundaries and to strengthen the theoretical foundations underlying these rapidly developing methodologies.

A central theme of the workshop was the interplay between geometric structure and approximation methods. Classical tools from approximation theory and numerical analysis often rely on linearity, while manifold-valued data inherently exhibit nonlinear behavior governed by curvature, topology, and global geometric constraints. The contributions addressed how such geometric features influence interpolation, regression, multiscale representations, extrapolation, and optimization, and how they can be systematically incorporated into algorithms via intrinsic constructions, tangent-space methods, or carefully designed extrinsic approaches. Particular attention was given to multiscale and hierarchical methods, kernel-based techniques, geometric finite element methods, and the role of curvature in error analysis and stability, among others.

The workshop combined survey-style lectures with presentations of new results and open problems, encouraging in-depth discussions among participants at different career stages. Applications provided a unifying perspective, illustrating how manifold-valued approximation arises naturally in areas such as signal and image processing, reduced-order modeling, data-driven scientific computing, and interpretable machine learning. A recurring conclusion of the discussions was the need for closer interaction between theory and practice: while applications continue to drive innovation, rigorous analysis remains essential for explainability, robustness, and long-term progress. By bringing together a diverse and growing community, the mini-workshop helped consolidate the field and identify promising directions for future research.

Mini-Workshop: Approximation of Manifold-Valued Functions

Table of Contents

Abstracts

A short introduction to Riemannian interpolation and a new Stiefel retraction with explicit inverse

Ralf Zimmermann

In this introductory talk to the mini-workshop on *Approximation of Manifold-Valued Functions*, we outlined basic concepts of Riemannian computing. Starting from the definitions of differentiable manifolds, matrix manifolds, Lie groups and quotient spaces, we exposed the role of geodesics as fundamental building blocks in Riemannian computing. As geodesics give rise to the Riemannian normal coordinates, they can be used as the Riemannian counterparts to the arithmetic operations of addition and subtraction in Riemannian manifolds. We also explored their relation to covariant derivatives and the impact of curvature on numerical algorithms on manifolds. Finally, we discussed the role of local coordinates in manifold interpolation applications and concluded the talk with two associated numerical examples.

Since all of the above is well known, I want to use this report to share an idea that took shape while being onsite at Oberwolfach. It is about a new way to compute local coordinates on the compact Stiefel manifold that can be considered a counterpart to the Grassmann coordinates from [4, Appendix C.4] that are further investigated in [5]. The idea sparked during discussions with Knut Hüper, Simon Mataigne and Rasmus Jensen during the workshop, although these were centered on the Grassmann case.

A new second-order Stiefel retraction with explicit inverse

Interpolation on manifolds typically relies on invertible local coordinates, most notably the Riemannian normal coordinates and their first-order approximations, called retractions [1, Section 4.1]. Consider the Stiefel manifold

$$St(n,p) = \{U \in \mathbb{R}^{n\times p} \mid U^T U = I_{p\times p}\}.$$

The dimension of the Stiefel manifold is $\frac{p}{2}(p-1) + (n-p)p$, which reflects the number of independent parameters in a skew-symmetric $(p \times p)$-matrix and a rectangular $(n-p) \times p$-matrix. Fix $\hat{U} \in St(n,p)$ with orthogonal completion $\hat{U}_\perp \in St(n, n-p)$. The tangent space at $\hat{U}$ is $T_{\hat{U}}St(n,p) = \{\xi = \hat{U}A + \hat{U}_\perp B \mid A \in \text{skew}(p), B \in \mathbb{R}^{(n-p)\times p}\}$.

A popular Stiefel retraction is the polar factor retraction: It reads

$$R_{\hat{U}} : T_{\hat{U}}St(n,p) \to St(n,p), \xi = \hat{U}A + \hat{U}_\perp B \mapsto (\hat{U} + \xi)\left(I_p + (A^T A + B^T B)\right)^{-\frac{1}{2}},$$

see [1, eq. (4.7)] and [2] for higher-order extensions. In its basic form, inversion requires solving a Lyapunov equation. Moreover, it relies on a polar decomposition of the full-size $(n \times p)$-matrix. Hence, for the sake of argument, we call it a *macro polar expression.*

A micro polar expression. Any Stiefel matrix can be split into sub-blocks $U = \begin{bmatrix} U_1 \\ U_2 \end{bmatrix}$ with $U_1 \in \mathbb{R}^{p\times p}$ and $U_2 \in \mathbb{R}^{(n-p)\times p}$. A local coordinate representation can be obtained from a polar decomposition of U_1 alone; hence the term *micro*. Assume that $\hat{U} = \begin{bmatrix} \hat{U}_1 \\ \hat{U}_2 \end{bmatrix} \in St(n,p)$ is fixed and features $\hat{U}_1$ invertible.[1] The map

$$\begin{aligned} \Psi : St(n,p) \supset \mathcal{B} \quad &\to \quad \mathrm{skew}(p) \times \mathbb{R}^{(n-p)\times p} \cong \mathbb{R}^{\frac{p}{2}(p-1)+(n-p)p} \\ U = \begin{bmatrix} U_1 \\ U_2 \end{bmatrix} \quad &\mapsto \quad \begin{bmatrix} \log_m\left(U_1(U_1^T U_1)^{-\frac{1}{2}}\right) \\ U_2(U_1^T U_1)^{-\frac{1}{2}} \end{bmatrix} =: \begin{bmatrix} A \\ B \end{bmatrix} \end{aligned}$$

is a coordinate chart on a suitable neighborhood $\mathcal{B}$ around $\hat{U}$. It can be computed as follows:

1: Compute a polar decomposition of the upper $(p \times p)$-block

$$U_1 = R\exp_m(X) = \exp_m(A)\exp_m(X),$$

where R is orthogonal, hence $A = \log_m(R)$ is skew-symmetric, and X is symmetric.

2: Set $B = U_2 \exp_m(X)^{-1}$.

3: Output: $\Psi(U) = (A, B)$.

The map Ψ is invertible; the inverse map $\varphi = \Psi^{-1}$ is a local paramaterization and is given by

$$\begin{aligned} \varphi : \mathrm{skew}(p) \times \mathbb{R}^{(n-p)\times p} \quad &\to \quad St(n,p), \\ \begin{bmatrix} A \\ B \end{bmatrix} \quad &\mapsto \quad \begin{pmatrix} \exp_m(A) \\ B \end{pmatrix} \sqrt{(I_{p\times p} + B^T B)^{-1}}. \end{aligned}$$

Since $(I_{p\times p} + B^T B)$ is symmetric positive definite, the inverse and the square root of the inverse are uniquely defined. A Taylor expansion shows that under the Euclidean metric, φ is a second-order retraction.

Details and further investigations are postponed to future work.

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[1] This assumption entails no essential restriction and can be enforced, if required, by a row perturbation. Alternatively, a block Householder QR as in [3, Sec. 5.1.7] can be used to transform any $U \in St(n,p)$ to the canonical representative $(I_{p\times p}, 0)^T \in St(n,p)$. We thank workshop participant Simon Mataigne for the latter observation.

Kernel-Based Methods for Scattered-Data Approximation

Holger Wendland

Kernel-based approximation methods represent a popular meshfree discretization technique. They are used in various areas comprising, for example, scattered data approximation [6], computer graphics, machine learning, aeroelasticity and the geosciences. They are closely related to support vector machines [5] and Gaussian processes [4].

The approximation space is formed as $V_X = \mathrm{span}\{K(\cdot, \mathbf{x}_1), \dots, K(\cdot, \mathbf{x}_N)\}$, using data sites $X = \{\mathbf{x}_1, \dots, \mathbf{x}_N\} \subseteq \mathcal{D} \subseteq \mathbb{R}^d$ and a fixed kernel function $K : \mathcal{D} \times \mathcal{D} \to \mathbb{R}$. This simple approach makes it easy to construct approximation spaces of arbitrary smoothness and in arbitrary dimensions.

In this talk, I gave a short introduction into the theory of kernel-based approximation methods, starting in the context of scalar-valued function approximation. Here, I discussed reproducing kernel Hilbert spaces $\mathcal{H}$ of functions $f : \mathcal{D} \to \mathbb{R}$ (see [1]) and the construction of a norm-minimal interpolant and a penalized least-squares approximant to such a function using only the discrete data $(X, f(X))$.

I discussed error estimates for target functions from Sobolev spaces $H^\sigma(\mathcal{D})$, using so-called sampling inequalities (see [3]) of the form

$$\|u\|_{W_q^m(\mathcal{D})} \le C \left(h_X^{\sigma - m - d(1/2 - 1/q)_+} \|u\|_{H^\sigma(\mathcal{D})} + h_X^{d/\max\{2,p,q\} - m} \|u(X)\|_p \right),$$

which give bounds on a lower-order Sobolev norm by a higher-order Sobolev norm and a discrete ℓ_p-norm employing the fill distance $h_X = \sup_{\mathbf{x} \in \mathcal{D}} \min_{\mathbf{x}_j \in X} \|\mathbf{x} - \mathbf{x}_j\|_2$.

After this, I then generalized these ideas to the approximation of Hilbert-space valued functions $f : \mathcal{D} \to W$, where W is another Hilbert space. The main ingredient for this is the generalization of the concept of a reproducing kernel Hilbert space $\mathcal{H} = \mathcal{H}(\mathcal{D}; W)$. Here, a kernel $K : \mathcal{D} \times \mathcal{D} \to L(W)$ has to map into the space $L(W)$ of all bounded and linear mappings from W to W. The kernel has to satisfy $K(\cdot, \mathbf{x})B \in \mathcal{H}$ for all $\mathbf{x} \in \mathcal{D}$ and all $B \in W$. Moreover, the reproduction property becomes

$$\langle f(\mathbf{x}), B \rangle_W = \langle f, K(\cdot, \mathbf{x})B \rangle_{\mathcal{H}},$$

for all $f \in \mathcal{H}(\mathcal{D}; W)$, $\mathbf{x} \in \mathcal{D}$ and $B \in W$.

Finally, I applied the latter theory to the manifold of positive definite and symmetric matrices $\mathbb{S}_n^+$ by employing a tangent space method to vectorize this manifold, see [2, 7].

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Manifold-valued function approximation from multiple tangent spaces

Hang Wang
(joint work with Raf Vandebril, Joeri Van der Veken and Nick Vannieuwenhoven)

We seek to approximate the—possibly unknown—function

$$f : \mathbb{R}^n \supset \Omega \longrightarrow \mathcal{M} \subset \mathbb{R}^m, \tag{1}$$

where Ω is open and $\mathcal{M}$ is an embedded *Riemannian submanifold* of $\mathbb{R}^m$, oftentimes equipped with the Euclidean metric from $\mathbb{R}^m$. We aim to find a function $\widehat{f} : \Omega \to \mathcal{M}$ that approximates f from N samples

$$S := \{(x_i, y_i) \in \Omega \times \mathcal{M} \mid i = 1, \ldots, N\}. \tag{2}$$

We make no assumptions on which samples S are provided to us: they could be (i) a fixed set of known input-output pairs as is common in machine learning; (ii) queried by the user from a given, usually expensive-to-evaluate function f; or (iii) a combination thereof.

Linearization constitutes an effective methodology for reducing manifold-valued function approximation to classic vector-valued function approximation, by pulling back the approximation problem to a single tangent space, as elucidated in [2, 8]. We refer to this technique as a *single tangent space model* (STSM). For now it suffices to clarify that STSM encompasses two principal stages. The first stage involves pulling back the outputs $\{y_1, \ldots, y_N\} \subset \mathcal{M}$ to a single *tangent space* $T_{p^*}\mathcal{M}$, where p^* is a designated *anchor point*, which could be, for example, an arbitrarily chosen point from $\{y_1, \ldots, y_N\}$ or their Fréchet mean.

The approximation models from [3, 4, 6] utilize a weighted Fréchet mean as the basis of an approximation of f. They can be thought of as generalizing the linear *moving least-squares method* [10] that approximates a function $f(x)$ between vector spaces by a linear combination of the outputs as $\widehat{f}(x) := \sum_{i=1}^N \varphi_i(x) y_i$, where φ_i are suitable weight functions, to the setting where the outputs y_i live on a Riemannian manifold. In these methods, proposed originally in [9, 3], the linear combination is substituted by a weighted Fréchet mean, resulting in the *Riemannian moving least squares* (RMLS) method. Recently, Sharon, Cohen, and Wendland [4] consider a multi-scale extension of RMLS, called MRMLS, which approximates the error of the previous scale with higher resolution samples using RMLS. A different extension was developed by Zimmermann and Bergmann [6]; they introduced the barycentric Hermite interpolation method that additionally interpolates the derivatives when computing the weighted Fréchet mean.

To address the limitation of locality in STSM and the high computational cost of the online stage of (multilevel) RMLS, we propose a new approach that unifies

STSM and RMLS. We call it the *multiple tangent spaces model* (MTSM). Our scheme utilizes multiple STSMs and combines their predictions with a weighted Fréchet mean. It can be thought of as replacing dense clusters of output samples by a single STSM. Hereby, MTSM can circumvent the locality restriction of STSM while significantly reducing the online computational cost of employing RMLS. MTSM trades off these advantages for a more costly offline stage.

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Interpolation on Riemannian Manifolds

Fátima Silva Leite

Solving interpolation problems on Riemannian manifolds efficiently has become an important research objective in recent years, due to their increasing interest in engineering fields such as robotics, computer vision, and signal and image processing, to name just a few.

In this talk, I have presented three different approaches for generating (cubic) splines on Riemannian manifolds, highlighting the advantages and disadvantages of each. The first two result from extending well-known procedures in Euclidean spaces to Riemannian manifolds in an intrinsic manner.

The first approach is a variational one, in which the interpolating curves are required to minimize the mean squared covariant acceleration. In this setting, the resulting curves are solutions of high-order nonlinear differential equations ([1], [2], [3]). Generalizations of this approach appeared recently in the survey paper [4].

The second approach uses the generalized de Casteljau algorithm, a geometric procedure based on successive geodesic interpolations. This method is theoretically appealing, but its practical implementation is often inefficient, since the resulting curves are defined by highly nonlinear implicit equations ([5]). Some comparison between the first two approaches appeared recently in [6].

The third approach is based on an extrinsic point of view. The Riemannian manifold on which the data lie is embedded isometrically into a Euclidean space, implying that all its (affine) tangent spaces embed into the same ambient space. A central role in this scheme is to project the data on the curved space to the affine tangent space at a chosen point by combining rolling the manifold over the flat space with additional time-dependent local diffeomorphisms. Rolling can be interpreted as a rigid motion subject to additional holonomic and non-holonomic constraints. The holonomic constraints ensure that, during the rolling motion, the manifold and the affine tangent space remain tangent along a prescribed curve on the manifold. The non-holonomic constraints prevent the manifold from spinning or sliding. Once the data have been transferred to the flat space, classical interpolation methods can be applied to generate a Euclidean spline, which is then mapped back to the manifold by the inverse operations. The result is an interpolating curve that is coordinate-free and available in closed form ([7], [8], [9]).

Comparison between the results from the three approaches is still under investigation. Numerical methods on manifolds have to be applied to obtain approximate solutions when no closed-form solutions are available.

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From Details to Horizons: Multiscale Approximation and Extrapolation

Nir Sharon

We study multiscale methods for approximation, analysis, and extrapolation of functions from scattered data, with particular emphasis on manifold-valued settings. This talk consists of two parts. The first part of the talk presents two complementary multiscale constructions: a bottom-up pyramid transform based on refinement and decimation operators, and a top-down multilevel scheme driven by quasi-interpolation. These frameworks provide stable hierarchical representations, yield decay estimates for multiscale coefficients, and enable feature detection, denoising, and anomaly identification. We illustrate the theory with applications to curves, rotation fields, and symmetric positive definite matrix fields.

The second part addresses the fundamental challenges of extrapolation from incomplete data. We discuss the inherent ill-posedness of extrapolation, analyze error propagation under limited prior information, and present recent approaches that mitigate error growth near domain boundaries. In particular, we introduce learning- and model-based strategies, including least-squares and rational extrapolation techniques, and demonstrate their performance through numerical examples. The results highlight both the power and the limitations of extrapolation, emphasizing the critical role of structural assumptions in achieving meaningful recovery beyond observed data.

Multiscale Analysis and Sparse Approximations of Manifold-Valued Data

Wael Mattar
(joint work with Nir Sharon)

Multiscale analysis has become a cornerstone of modern signal and image processing. Driven by the objective of representing data in a hierarchical fashion, capturing coarse-to-fine structures and revealing features across scales, multiscale transforms enable powerful techniques for a wide range of applications. In this talk, we will begin with a comprehensive overview of the construction of multiscale transforms via refinement operators, highlighting recent advances in the area. These operators serve as upsampling in the process of multiscaling. Once established, we will describe the adaptation of multiscale transforms to the multivariate setting, as well as to manifold-valued data, and then focus on the optimization problem of sparse approximations. Lastly, we will discuss the extension of multiscale transforms to Wasserstein spaces and present a few applications in this setting. The talk will highlight both theoretical developments and practical implementations, illustrating the potential of multiscale methods in emerging data-driven applications.

On the approximation of the Riemannian barycenter

Simon Mataigne

We present a method for computing an approximate Riemannian barycenter of a collection of points lying on a Riemannian manifold. Our approach relies on the use of theoretically proven under- and over-approximations of the Riemannian distance function. We compare it to Riemannian steepest descent on the exact objective function of the Riemannian barycenter and to an approach that approximates the Riemannian logarithm using lifting maps. Experiments are conducted on the Stiefel manifold. We also present a novel method for computing the eigenvalue decomposition of an orthogonal matrix. This method relies on the eigenvalue decomposition of the skew-symmetric part.

Maximum volume coordinates for Grassmann interpolation: Lagrange, Hermite, and errors

Rasmus Jensen

A unified framework for studying extremal curves on real Stiefel manifolds is presented. We start with a smooth one-parameter family of pseudo-Riemannian metrics on a product of orthogonal groups acting transitively on Stiefel manifolds. In the next step Euler-Langrange equations for a whole class of extremal curves on Stiefel manifolds are derived. This includes not only geodesics with respect to different Riemannian metrics, but so-called quasi-geodesics and smooth curves of constant geodesic curvature, as well. It is shown that they all can be written in closed form.This is verified by studying the solutions of a linear, second order, explicit, matrix-valued ordinary differential equation and an associated initial value problem.

Our results are put into perspective to recent work where certain numerical schemes for solving the socalled endpoint geodesic problem on the Stiefel manifold has been discussed. Moreover, beyond our unifying approach, for some specific values of the parameter we recover certain well-known results from the literature.

A Lagrangian approach to extremal curves on Stiefel manifolds

Knut Hüper

This talk presents a Riemannian framework for interpretable machine learning that turns the manifold hypothesis into a concrete geometric pipeline: learning a global Riemannian structure, extracting geodesic submanifolds, and solving downstream optimization tasks on these learned manifolds. The central theme is that by working with pullback and iso-Riemannian geometries, one can retain closed-form manifold mappings, control geodesic speed, and recover Euclidean-like optimization guarantees while operating on highly non-linear data manifolds.

Locally Isometric Embeddings of Quotients of the Rotation Group

Ralf Hielscher

Quotients $SO(3)/S$ of the rotation group $SO(3)$ with respect to finite symmetry groups $S \subset SO(3)$ play an important role in crystallography, robotics, and molecular science. Although the analysis of manifold-valued data has seen big progressions during the last years, there are still many methods that are only applicable to data in Euclidean vector spaces. For this reason we are interested in embeddings of the quotients $SO(3)/S$ into some vector space $\mathbb{R}^d$. According to the Nash embedding theorem, such embeddings exist for $d \geq 15$. In order to explicitly construct isometric embeddings of $SO(3)/S$, we analyse their spectral embeddings. In the talk, we report on the global properties of isometric embeddings found following this approach.

Geometric Finite Element

Hanne Hardering

Constrained minimization problems whose solutions take values in a Riemannian manifold motivate the development of geometric finite element methods. These methods are designed to be independent of embeddings, invariant under manifold isometries, and to coincide with classical finite elements when the target space is $\mathbb{R}^n$.

To achieve this, manifold-valued polynomials are defined on each element of the grid using intrinsic interpolation methods. Geometric finite elements are then defined as continuous maps whose restrictions to each element are such polynomials. The two interpolation methods that have been used in this context so far are a Riemannian center-of-mass construction weighted by Lagrangian basis functions, and the closest-point projection of interpolants defined in an ambient space $\mathbb{R}^{n+1}$. To measure classical interpolation and discretization errors, intrinsic smoothness descriptors and intrinsic Sobolev distances are employed. With these tools, manifold-valued maps exhibit the behavior expected from the Euclidean case with respect to the grid-width parameter, although analogues of full Sobolev norms, rather than seminorms, appear on the right-hand side of the estimates.

The method described in particular generalizes Lagrangian finite elements, where discrete interpolation is defined using point values of a continuous function. Consequently, interpolation is restricted to continuous functions and exhibits the characteristic stability properties of Lagrangian interpolation operators. In the finite element context, however, it is often useful to consider alternative elements that do not rely on nodal values. This talk presents a possible construction of a manifold-valued Scott–Zhang-type interpolation operator, establishes corresponding stability estimates, and outlines ideas for the proof of interpolation error estimates.

Kernel-based Interpolation of Manifold-Valued Functions

Daniel Fischer

Radial basis function (RBF) interpolation is a widely used technique for reconstructing functions from their values at scattered data sites. While RBF interpolation of functions defined on manifolds is well understood, the interpolation of manifold-valued functions by RBFs has received far less attention. In this talk, I will describe how RBF interpolation can be combined with three standard approaches to manifold-valued interpolation, namely interpolation via embedding and projection, interpolation via tangent spaces, and interpolation via Riemannian means. I will focus on deriving error estimates analogous to those in the classical theory and illustrate these results with numerical examples.

Subdivision Schemes: from Manifolds to Metric Spaces

Nira Dyn
(joint work with Nir Sharon)

This talk consists of three parts.

The first part is a short overview of "classical" results on univariate, linear Subdivision Schemes, refining sequences of points in Euclidean Spaces. Special emphasis is given to B-spline schemes and the Lane-Riesenfeld (L-R) algorithm for their computation. Basic notions such as the convergence of a subdivision scheme are defined, and a necessary condition for convergence is stated.

The second part discusses the adaptation of B-spline schemes to manifold-valued point sequences using the L-R algorithm. This is done by replacing the Arithmetic average between two Euclidean points with the Geodesic average between two points in a manifold. This result appears in a joint paper with Nir published in 2017, where the "Global approach" (a generalization of the L-R algorithm) is applied to a wide family of univariate linear subdivision schemes, allowing the adaptation of these schemes to manifold-valued data, based on the weighted "geodesic average".

The third part addresses subdivision schemes operating on elements of a metric space. First, the notion of a binary average of such elements is defined. Then it is used in the definition of refinement of sequences of such elements, with the binary average replacing the arithmetic average in the L-R algorithm. Also, the notion of convergence of subdivision schemes is based on the binary average.

Three examples of metric spaces where subdivision schemes have already been studied are presented: the metric space with elements the non-empty compact subsets of $\mathbb{R}^d$ with the Hausdorff metric, the Wasserstein space and the space of "geometric Hermit pairs", each consisting of a point and a unit tangent vector, namely the metric space $\mathbb{R}^d \times \mathbb{S}^{d-1}$ endowed with a corresponding product metric. These results, along with others, appear in a joint paper with Nir, which was recently submitted for publication.

Riemannian geometry for interpretable machine learning

Willem Diepeveen

This talk presents a Riemannian framework for interpretable machine learning that turns the manifold hypothesis into a concrete geometric pipeline: learning a global Riemannian structure, extracting geodesic submanifolds, and solving downstream optimization tasks on these learned manifolds. The central theme is that by working with pullback and iso-Riemannian geometries, one can retain closed-form manifold mappings, control geodesic speed, and recover Euclidean-like optimization guarantees while operating on highly non-linear data manifolds.

Approximation of Manifold-Valued Functions

Jonas Bresch
(joint work with Robert Beinert and Gabriele Steidl)

Reconstruction and denoising manifold-valued data is a common task in many applications. Different tasks require different data representations encoded naturally in several manifolds.

Phase and orientation measurements, *chromaticity* components of color images, and statistical pixel descriptors are commonplace areas for manifold-valued data. Circle-valued data arise in *interferometric synthetic aperture radar* (ISAR) in color restoration models based on the *hue-saturation-value* (HSV) or *lightness-chromaticity-hue* (LCh) color spaces, and in phase imaging for *magnetic resonance.* 3d-sphere-valued signals model directional data arising in 3d orientation and directional sensing problems and appear in *chromaticity-brightness* image models. The *special orthogonal group* (SO) encodes rotations and arises in motion analysis and *electron back-scatter diffraction* (EBSD) imaging while quaternion representations are sometimes used for color and orientation processing. In another direction, the Fisher-metric geometry of Gaussian distributions identifies a two-dimensional hyperbolic sheet as a natural manifold for pixelwise mean–variance models, connecting probabilistic image models to hyperbolic-geometry-based processing. Generalizing the $(d-1)$-dimensional sphere yields the Stiefel-manifold, which arises in many applications, for instance, in image and video-based recognition and for handling orthonormal constraints. Beyond "classical" manifold-valued data, multi-binary valued data, as generalization of binary-valued data, can be found in modern and secure information transmission systems, for instance in multi-colour *quick-response* (QR) codes. Instead of black and white QR codes—two-dimensional matrix barcodes (invented in 1994 by Hara)—the color channels in the RGB values (red-blue-green) are added to the color model yielding modules in black, red, blue, green, cyan, magenta, yellow, and white.

All these quite different applications motivate to formulate a unifite pathway for all the different underlying manifolds. The aim is to be as manifold- and geometry-aware as necessary but, on the other side, as relaxed as possible allowing the application of state-of-the-art solver from convex analysis with existing convergence guarantees.

For doing so, novel GRAM matrix representations $\boldsymbol{Q}$ for the manifold-valued data are proposed via a *positive semidefinite* lifting including minimal rank constraints. Those are the nonconvex constraints from the manifold originating due to the EUCLIDEAN embedding of the considered manifolds ensured by WHITNEY's (strong) embedding theorem for any smooth real m-dimensional manifold.

There are two different regularizer considered: the squared TIKHONOV and TOTAL VARIATION (TV) regularization. Therefore, the following nonconvex optimization problem is aimed to solve:

$$\arg\min_{\boldsymbol{x}\in\mathbb{M}^N} \sum_{n\in V} \tfrac{w_n}{2}\|\boldsymbol{x}_n-\boldsymbol{y}_n\|_2^2 + \sum_{(n,m)\in E} \lambda_{(n,m)}\mathcal{D}(\boldsymbol{x}_n,\boldsymbol{x}_m), \tag{1}$$

where $\mathbb{M} \hookrightarrow \mathbb{R}^{d_\mathbb{M}}$ is the ambient EUCLIDEAN embedding with underlying data structure, given by a connected, undirected graph $G=(V,E)$ with $|V| \coloneqq N$ and $|E| \coloneqq M$. The chosen penalizers $\mathcal{D}: \mathbb{R}^{d_\mathbb{M}} \times \mathbb{R}^{d_\mathbb{M}} \to \mathbb{R}$ are

$$\mathcal{D}(\cdot^1,\cdot^2) \in \{\|\cdot^1-\cdot^2\|_1, {}^1\!/_2\|\cdot^1-\cdot^2\|_2^2\},$$

i.e. the Manhattan and the (squared) EUCLIDEAN norm. Capturing both regularizers enables to handle smooth and non-smooth, i.e., e.g. piecewise constant, data. It holds [4, 3, 1, 2]

$$(1) = \operatorname*{arg\,min}_{\substack{\boldsymbol{x}\in\mathbb{R}^{d_\mathbb{M}}\\ \boldsymbol{v}\in\mathbb{R}^N,\boldsymbol{\ell}\in\mathbb{R}^M}} \sum_{n\in V} \tfrac{w_n}{2}(\boldsymbol{v}_n - 2\langle \boldsymbol{x}_n,\boldsymbol{y}_n\rangle) + \sum_{(n,m)\in E}\lambda_{(n,m)}\mathcal{D}(\boldsymbol{x}_n,\boldsymbol{x}_m) =: \mathcal{K}(\boldsymbol{x},\boldsymbol{v},\boldsymbol{\ell}),$$

$$\text{s.t.} \quad \begin{cases} \boldsymbol{Q}_{(n,m)}(\boldsymbol{x},\boldsymbol{v},\boldsymbol{\ell}) \succcurlyeq \boldsymbol{0}, \\ \min \operatorname{rk}(\boldsymbol{Q}_{(n,m)}(\boldsymbol{x},\boldsymbol{v},\boldsymbol{\ell})), \end{cases} \qquad \forall (n,m)\in E. \tag{2}$$

Here, $\boldsymbol{v}_n$ parametrizes $\|\boldsymbol{x}_n\|^2$ and $\boldsymbol{\ell}_{(n,m)}$ parametrizes $\langle \boldsymbol{x}_n,\boldsymbol{x}_m\rangle$. It is proposed [4, 3, 1, 2] to neglect the rank constraints in (2) and to solve instead the

convex relaxed model

$$\operatorname*{arg\,min}_{\substack{\boldsymbol{x}\in\mathbb{R}^{d_\mathbb{M}}\\ \boldsymbol{v}\in\mathbb{R}^N,\boldsymbol{\ell}\in\mathbb{R}^M}} \mathcal{K}(\boldsymbol{x},\boldsymbol{v},\boldsymbol{\ell}) \quad \text{s.t.} \quad \boldsymbol{Q}_{(n,m)}(\boldsymbol{x},\boldsymbol{v},\boldsymbol{\ell}) \succcurlyeq \boldsymbol{0} \quad \forall (n,m)\in E. \tag{3}$$

If the squared EUCLIDEAN norm is used, the function $\mathcal{K}(\boldsymbol{x},\boldsymbol{v},\boldsymbol{\ell})$ becomes linear in all components [4, 1, 2], due to

$$\|\boldsymbol{x}_n-\boldsymbol{x}_m\|_2^2 = \boldsymbol{v}_n + \boldsymbol{x}_m - 2\boldsymbol{\ell}_{(n,m)}.$$

Beyond theoretical *tightness results* for $\mathbb{M}=\mathbb{S}_0^d$ [3, 2], i.e. multi-ninary-valued data, meaning that solutions of (3) can be used to obtain global solutions of the original nonconvex optimization problem (1), the computational examples [4, 3, 1, 2] admit across all experiments such a behavior and, more precisely, the computed solution are already manifold-valued.

References

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Nonsmooth Optimization on Riemannian Manifolds

Ronny Bergmann

In many applications nonlinear data is measured, for example when considering unit vectors $\{p \in \mathbb{R}^n \,\|\, \|p\| = 1\}$, rotations $\{p \in \mathbb{R}^{n\times n} \,|\, p^\top p = I, \det p = 1\}$, symmetric positive definite matrices $\mathcal{P}(n) := \{p \in \mathbb{R}^{n\times n} \,|\, p = p^\top, x^\top px > 0 \text{ for all } x \neq 0\}$, or (bases of) subspaces of a vector space, the Stiefel and Grassmann manifold, respectively. Modelling this on a Riemannian manifold allows to both reduce the dimension of the data stored as well as focusing on geometric properties of the measurement space compared to constraining a total space the data is represented in. In optimisation this yields unconstrained optimization algorithms, where we obtain that every iterate is a feasible point, but we have to take the geometry of the optimization domain into consideration.

In this talk we present recent developments in nonsmooth optimization on manifolds. We consider optimization problems of the form

$$\operatorname*{arg\,min}_{p\in\mathcal{M}} f(p),$$

where $\mathcal{M}$ is a Riemannian manifold and $f\colon \mathcal{M} \to \mathbb{R}$ is a cost function. One challenge is that the manifold might be high-dimensional, e.g.hen considering images in diffusion tensor imaging, where each pixel is represented by a symmetric positive definite matrix, and hence we obtain the manifold $\mathcal{P}(3)^{m\times n}$ for an $m \times n$ image. Another challenge is that the cost function f might be nonsmooth, and we hence can not apply quasi Newton other Hessian or gradient based methods.

The main scheme we present is based on splitting methods, where the cost function f can be written as a sum of several functions, each with certain properties. Starting from the well-known proximal point algorithm, we consider the Cyclic Proximal Point Algorithm (CPPA) that is based on a cyclic evaluation of the proximal mappings when f can be written as a sum of several functions.

Further, we present extensions of the Douglas-Rachford algorithm for the case when $f = g+h$ is a sum of two proper convex lower semicontinuous (lsc.) functions, as well as extension of the Fenchel conjugate and the Chambolle-Pock algorithm to the Riemannian setting. This can be further used to define a Riemannian version of the Primal-Dual Semismooth Newton.

As a final algorithm we present a Riemannian extension of the well-known Difference of convex algorithm, where the objective function $f = g - h$ can be written as a difference of two proper convex lsc. functions.

We will present the packages `ManifoldsBase.jl`, an abstract interface for Riemannian manifolds in Julia, `Manifolds.jl`, a package providing various Riemannian manifolds based on that interface, and `Manopt.jl`, a package for optimization on Riemannian manifolds that defines algorithms on general Riemannian manifolds also based on the interface. These include all of the presented algorithms above.

Numerical examples finally both illustrate the performance as well as the ease of use of the presented algorithms within the software packages.

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Participants

Prof. Dr. Ronny Bergmann
Department of Mathematical Sciences
Norwegian University of Science and Technology
7491 Trondheim
NORWAY

Jonas Bresch
Institut für Mathematik
TU Berlin
Str. des 17. Juni 136
10587 Berlin
GERMANY

Willem Diepeveen
UCLA
Department of Mathematics
520 Portola Plaza
P.O. Box 951438
Los Angeles, CA 90095-1438
UNITED STATES

Prof. Dr. Nira Dyn
School of Mathematical Sciences
Tel Aviv University
Ramat Aviv
Tel Aviv 69978
ISRAEL

Daniel Fischer
Mathematisches Institut
Universität Bayreuth
95447 Bayreuth
GERMANY

Dr. Hanne Hardering
Institut für Numerische Mathematik
Fachrichtung Mathematik
Technische Universität Dresden
01062 Dresden
GERMANY

Ralf Hielscher
Fakultät für Mathematik
und Informatik
Technische Universität
Bergakademie Freiberg
Prüferstr. 1
09599 Freiberg
GERMANY

Prof. Dr. Knut Hüper
Institut für Mathematik
Universität Würzburg
Emil-Fischer-Straße 31
97074 Würzburg
GERMANY

Rasmus Jensen
Department of Mathematics and
Computer Science
University of Southern Denmark
Campusvej 55
5230 Odense M
DENMARK

Simon Mataigne
ICTEAM Institute
Université Catholique de Louvain
Avenue Georges Lemaitre 4
1348 Louvain-la-Neuve
BELGIUM

Wael Mattar
Department of Mathematics
School of Mathematical Sciences
Tel Aviv University
Ramat Aviv
Tel Aviv 69978
ISRAEL

Prof. Dr. Nir Sharon
Department of Mathematics
School of Mathematical Sciences
Tel Aviv University
Ramat Aviv
Tel Aviv 69978
ISRAEL

Prof. Dr. Fatima Silva Leite
Institute of Systems and Robotics
Universidade de Coimbra
R. Silvio Lima
3030-290 Coimbra
PORTUGAL

Hang Wang
KU Leuven
Celestijnenlaan 200A
P.O. Box bus 2402
3001 Leuven
BELGIUM

Prof. Dr. Holger Wendland
Mathematisches Institut
Universität Bayreuth
95440 Bayreuth
GERMANY

Prof. Dr. Ralf Zimmermann
Institut for Matematik og Datalogi
Syddansk Universitet
Campusvej 55
5230 Odense M
DENMARK