Transformations Based on Continuous Piecewise-Affine Velocity Fields

We propose novel finite-dimensional spaces of well-behaved transformations. The latter are obtained by (fast and highly-accurate) integration of continuous piecewise-affine velocity fields. The proposed method is simple yet highly expressive, effortlessly handles optional constraints (e.g., volume preservation and/or boundary conditions), and supports convenient modeling choices such as smoothing priors and coarse-to-fine analysis. Importantly, the proposed approach, partly due to its rapid likelihood evaluations and partly due to its other properties, facilitates tractable inference over rich transformation spaces, including using Markov-Chain Monte-Carlo methods. Its applications include, but are not limited to: monotonic regression (more generally, optimization over monotonic functions); modeling cumulative distribution functions or histograms; time-warping; image warping; image registration; real-time diffeomorphic image editing; data augmentation for image classifiers. Our GPU-based code is publicly available.
A locally adaptive normal distribution

The multivariate normal density is a monotonic function of the distance to the mean, and its ellipsoidal shape is due to the underlying Euclidean metric. We suggest to replace this metric with a locally adaptive, smoothly changing (Riemannian) metric that favors regions of high local density. The resulting locally adaptive normal distribution (LAND) is a generalization of the normal distribution to the "manifold" setting, where data is assumed to lie near a potentially low-dimensional manifold embedded in RD. The LAND is parametric, depending only on a mean and a covariance, and is the maximum entropy distribution under the given metric. The underlying metric is, however, non-parametric. We develop a maximum likelihood algorithm to infer the distribution parameters that relies on a combination of gradient descent and Monte Carlo integration. We further extend the LAND to mixture models, and provide the corresponding EM algorithm. We demonstrate the efficiency of the LAND to fit non-trivial probability distributions over both synthetic data, and EEG measurements of human sleep.

General information

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Authors: Arvanitidis, G. (Intern), Hansen, L. K. (Intern), Hauberg, S. (Intern)
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Electroencephalography (EEG) is a flexible and accessible tool with excellent temporal resolution but with a spatial resolution hampered by volume conduction. Reconstruction of the cortical sources of measured EEG activity partly alleviates this problem and effectively turns EEG into a brain imaging device. The quality of the source reconstruction depends on the forward model which details head geometry and conductivities of different head compartments. These person-specific factors are complex to determine, requiring detailed knowledge of the subject’s anatomy and physiology. In this proof-of-concept study, we show that, even when anatomical knowledge is unavailable, a suitable forward model can be estimated directly from the EEG. We propose a data-driven approach that provides a low-dimensional parametrization of head geometry and compartment conductivities, built using a corpus of forward models. Combined with only a recorded EEG signal, we are able to estimate both the brain sources and a person-specific forward model by optimizing this parametrization. We thus not only solve an inverse problem, but also optimize over its specification. Our work demonstrates that personalized EEG brain imaging is possible, even when the head geometry and conductivities are unknown.
Forward Models can be Inferred from EEG Data

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Open Problem: Kernel methods on manifolds and metric spaces: What is the probability of a positive definite geodesic exponential kernel?
Radial kernels are well-suited for machine learning over general geodesic metric spaces, where pairwise distances are often the only computable quantity available. We have recently shown that geodesic exponential kernels are only positive definite for all bandwidths when the input space has strong linear properties. This negative result hints that radial kernels are perhaps not suitable over geodesic metric spaces after all. However, we present evidence that large intervals of bandwidths exist where geodesic exponential kernels have high probability of being positive definite over finite datasets, while still having significant predictive power. From this we formulate conjectures on the probability of a positive definite kernel matrix for a finite random sample, depending on the geometry of the data space and the spread of the sample.

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Organisations: Department of Applied Mathematics and Computer Science, Cognitive Systems, University of Copenhagen
Authors: Feragen, A. (Ekstern), Hauberg, S. (Intern)
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Scalable Robust Principal Component Analysis Using Grassmann Averages
In large datasets, manual data verification is impossible, and we must expect the number of outliers to increase with data size. While principal component analysis (PCA) can reduce data size, and scalable solutions exist, it is well-known that outliers can arbitrarily corrupt the results. Unfortunately, state-of-the-art approaches for robust PCA are not scalable. We note that in a zero-mean dataset, each observation spans a one-dimensional subspace, giving a point on the Grassmann manifold. We show that the average subspace corresponds to the leading principal component for Gaussian data. We provide a simple algorithm for computing this Grassmann Average (GA), and show that the subspace estimate is less sensitive to outliers than PCA for general distributions. Because averages can be efficiently computed, we immediately gain scalability. We exploit robust averaging to formulate the Robust Grassmann Average (RGA) as a form of robust PCA. The resulting Trimmed Grassmann Average (TGA) is appropriate for computer vision because it is robust to pixel outliers. The algorithm has linear computational complexity and minimal memory requirements. We demonstrate TGA for background modeling, video restoration, and shadow removal. We show scalability by performing robust PCA on the entire Star Wars IV movie; a task beyond any current method. Source code is available online.

General information
A Random Riemannian Metric for Probabilistic Shortest-Path Tractography

Shortest-path tractography (SPT) algorithms solve global optimization problems defined from local distance functions. As diffusion MRI data is inherently noisy, so are the voxelwise tensors from which local distances are derived. We extend Riemannian SPT by modeling the stochasticity of the diffusion tensor as a "random Riemannian metric", where a geodesic is a distribution over tracts. We approximate this distribution with a Gaussian process and present a probabilistic numerics algorithm for computing the geodesic distribution. We demonstrate SPT improvements on data from the Human Connectome Project.

Geodesic exponential kernels: When Curvature and Linearity Conflict

We consider kernel methods on general geodesic metric spaces and provide both negative and positive results. First we show that the common Gaussian kernel can only be generalized to a positive definite kernel on a geodesic metric space if the space is flat. As a result, for data on a Riemannian manifold, the geodesic Gaussian kernel is only positive definite if the Riemannian manifold is Euclidean. This implies that any attempt to design geodesic Gaussian kernels on curved Riemannian manifolds is futile. However, we show that for spaces with conditionally negative definite distances the geodesic Laplacian kernel can be generalized while retaining positive definiteness. This implies that geodesic Laplacian kernels can be generalized to some curved spaces, including spheres and hyperbolic spaces. Our theoretical results are verified empirically.
Highly-Expressive Spaces of Well-Behaved Transformations: Keeping It Simple

We propose novel finite-dimensional spaces of $\mathbb{R}^n \to \mathbb{R}^n$ transformations, $n \in \{1, 2, 3\}$, derived from (continuously-defined) parametric stationary velocity fields. Particularly, we obtain these transformations, which are diffeomorphisms, by fast and highly-accurate integration of continuous piecewise-affine velocity fields; we also provide an exact solution for $n = 1$. The simple-yet-highly-expressive proposed representation handles optional constraints (e.g., volume preservation) easily and supports convenient modeling choices and rapid likelihood evaluations (facilitating tractable inference over latent transformations). Its applications include, but are not limited to: unconstrained optimization over monotonic functions; modeling cumulative distribution functions or histograms; time warping; image registration; landmark-based warping; real-time diffeomorphic image editing.

On Geodesic Exponential Kernels

This extended abstract summarizes work presented at CVPR 2015 [1].

Standard statistics and machine learning tools require input data residing in a Euclidean space. However, many types of data are more faithfully represented in general nonlinear metric spaces or Riemannian manifolds, e.g. shapes, symmetric positive definite matrices, human poses or graphs. The underlying metric space captures domain specific knowledge, e.g. non-linear constraints, which is available a priori. The intrinsic geodesic metric encodes this knowledge, often leading to improved statistical models.
Principal Curves on Riemannian Manifolds

Euclidean statistics are often generalized to Riemannian manifolds by replacing straight-line interpolations with geodesic ones. While these Riemannian models are familiar-looking, they are restricted by the inflexibility of geodesics, and they rely on constructions which are optimal only in Euclidean domains. We consider extensions of Principal Component Analysis (PCA) to Riemannian manifolds. Classic Riemannian approaches seek a geodesic curve passing through the mean that optimize a criteria of interest. The requirements that the solution both is geodesic and must pass through the mean tend to imply that the methods only work well when the manifold is mostly flat within the support of the generating distribution. We argue that instead of generalizing linear Euclidean models, it is more fruitful to generalize non-linear Euclidean models. Specifically, we extend the classic Principal Curves from Hastie & Stuetzle to data residing on a complete Riemannian manifold. We show that for elliptical distributions in the tangent of spaces of constant curvature, the standard principal geodesic is a principal curve. The proposed model is simple to compute and avoids many of the pitfalls of traditional geodesic approaches. We empirically demonstrate the effectiveness of the Riemannian principal curves on several manifolds and datasets.
As the collection of large datasets becomes increasingly automated, the occurrence of outliers will increase—"big data" implies "big outliers". While principal component analysis (PCA) is often used to reduce the size of data, and scalable solutions exist, it is well-known that outliers can arbitrarily corrupt the results. Unfortunately, state-of-the-art approaches for robust PCA do not scale beyond small-to-medium sized datasets. To address this, we introduce the Grassmann Average (GA), which expresses dimensionality reduction as an average of the subspaces spanned by the data. Because averages can be efficiently computed, we immediately gain scalability. GA is inherently more robust than PCA, but we show that they coincide for Gaussian data. We exploit that averages can be made robust to formulate the Robust Grassmann Average (RGA) as a form of robust PCA. Robustness can be with respect to vectors (subspaces) or elements of vectors; we focus on the latter and use a trimmed average. The resulting Trimmed Grassmann Average (TGA) is particularly appropriate for computer vision because it is robust to pixel outliers. The algorithm has low computational complexity and minimal memory requirements, making it scalable to "big noisy data." We demonstrate TGA for background modeling, video restoration, and shadow removal. We show scalability by performing robust PCA on the entire Star Wars IV movie.
Metrics for Probabilistic Geometries
We investigate the geometrical structure of probabilistic generative dimensionality reduction models using the tools of Riemannian geometry. We explicitly define a distribution over the natural metric given by the models. We provide the necessary algorithms to compute expected metric tensors where the distribution over mappings is given by a Gaussian process. We treat the corresponding latent variable model as a Riemannian manifold and we use the expectation of the metric under the Gaussian process prior to define interpolating paths and measure distance between latent points. We show how distances that respect the expected metric lead to more appropriate generation of new data.

Model Transport: Towards Scalable Transfer Learning on Manifolds
We consider the intersection of two research fields: transfer learning and statistics on manifolds. In particular, we consider, for manifold-valued data, transfer learning of tangent-space models such as Gaussians distributions, PCA, regression, or classifiers. Though one would hope to simply use ordinary Rn-transfer learning ideas, the manifold structure prevents it.
We overcome this by basing our method on inner-product-preserving parallel transport, a well-known tool widely used in other problems of statistics on manifolds in computer vision. At first, this straightforward idea seems to suffer from an obvious shortcoming: Transporting large datasets is prohibitively expensive, hindering scalability. Fortunately, with our approach, we never transport data. Rather, we show how the statistical models themselves can be transported, and prove that for the tangent-space models above, the transport “commutes” with learning. Consequently, our compact framework, applicable to a large class of manifolds, is not restricted by the size of either the training or test sets. We demonstrate the approach by transferring PCA and logistic-regression models of real-world data involving 3D shapes and image descriptors.

**General information**
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Cognitive Systems, Max Planck Institute, Massachusetts Institute of Technology
Authors: Freifeld, O. (Ekstern), Hauberg, S. (Intern), Black, M. J. (Ekstern)
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**Probabilistic shortest path tractography in DTI using Gaussian Process ODE solvers**
Tractography in diffusion tensor imaging estimates connectivity in the brain through observations of local diffusivity. These observations are noisy and of low resolution and, as a consequence, connections cannot be found with high precision. We use probabilistic numerics to estimate connectivity between regions of interest and contribute a Gaussian Process tractography algorithm which allows for both quantification and visualization of its posterior uncertainty. We use the uncertainty both in visualization of individual tracts as well as in heat maps of tract locations. Finally, we provide a quantitative evaluation of different metrics and algorithms showing that the adjoint metric [8] combined with our algorithm produces paths which agree most often with experts.

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Organisations: Department of Applied Mathematics and Computer Science, Cognitive Systems, Max Planck Institute, University of Copenhagen
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Probabilistic Solutions to Differential Equations and their Application to Riemannian Statistics

We study a probabilistic numerical method for the solution of both boundary and initial value problems that returns a joint Gaussian process posterior over the solution. Such methods have concrete value in the statistics on Riemannian manifolds, where nonanalytic ordinary differential equations are involved in virtually all computations. The probabilistic formulation permits marginalising the uncertainty of the numerical solution such that statistics are less sensitive to inaccuracies. This leads to new Riemannian algorithms for mean value computations and principal geodesic analysis. Marginalisation also means results can be less precise than point estimates, enabling a noticeable speedup over the state of the art. Our approach is an argument for a wider point that uncertainty caused by numerical calculations should be tracked throughout the pipeline of machine learning algorithms.

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Projects:

Deep Metric Learning

Department of Applied Mathematics and Computer Science
Period: 01/09/2017 → 31/08/2020
Number of participants: 3
Phd Student:
Detlefsen, Nicki Skafte (Intern)
Supervisor:
Winther, Ole (Intern)
Main Supervisor:
Hauberg, Søren (Intern)

Financing sources
Source: Internal funding (public)
**The stochastic geometry of latent variable models**

Department of Applied Mathematics and Computer Science  
Period: 01/09/2017 → 31/08/2020  
Number of participants: 3  
Phd Student:  
Jørgensen, Martin (Intern)  
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Main Supervisor:  
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**Financing sources**  
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**Geometrical aspects of manifold learning**

Department of Applied Mathematics and Computer Science  
Period: 01/12/2015 → 30/11/2018  
Number of participants: 3  
Phd Student:  
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Supervisor:  
Hauberg, Søren (Intern)  
Main Supervisor:  
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