Intrinsic Gaussian Process on Unknown Manifolds with Probabilistic Metrics

Mu Niu, Zhenwen Dai, Pokman Cheung, Yizhu Wang

JMLR

Home Page
Papers
Submissions
News
Editorial Board
Special Issues
Open Source Software
Proceedings (PMLR)

Intrinsic Gaussian Process on Unknown Manifolds with Probabilistic Metrics

Mu Niu, Zhenwen Dai, Pokman Cheung, Yizhu Wang; 24(104):1−42, 2023.

Abstract

This article presents a novel approach to construct Intrinsic Gaussian Processes for regression on unknown manifolds with probabilistic metrics (GPUM) in point clouds. In many real world applications, one often encounters high dimensional data (e.g.‘point cloud data’) centered around some lower dimensional unknown manifolds. The geometry of manifold is in general different from the usual Euclidean geometry. Naively applying traditional smoothing methods such as Euclidean Gaussian Processes (GPs) to manifold-valued data and so ignoring the geometry of the space can potentially lead to highly misleading predictions and inferences. A manifold embedded in a high dimensional Euclidean space can be well described by a probabilistic mapping function and the corresponding latent space. We investigate the geometrical structure of the unknown manifolds using the Bayesian Gaussian Processes latent variable models(B-GPLVM) and Riemannian geometry. The distribution of the metric tensor is learned using B-GPLVM. The boundary of the resulting manifold is defined based on the uncertainty quantification of the mapping. We use the probabilistic metric tensor to simulate Brownian Motion paths on the unknown manifold. The heat kernel is estimated as the transition density of Brownian Motion and used as the covariance functions of GPUM. The applications of GPUM are illustrated in the simulation studies on the Swiss roll, high dimensional real datasets of WiFi signals and image data examples. Its performance is compared with the Graph Laplacian GP, Graph Mat\'{e}rn GP and Euclidean GP.

[abs][pdf][bib]

Outline

- Setup and Motivation
- Methods
- Result
- Conclusion

Set up and Motivation

- **Problem: Performing regression on unknown manifolds when dealing with high-dimensional data, particularly point cloud data.**

$$y_i = f(s_i) + \epsilon_i, \quad \epsilon_i \sim \mathcal{N}(0, \sigma_\epsilon^2)$$

- **Challenge**:
- Traditional methods, particularly Euclidean GPs, may produce misleading results due to a mismatch with intrinsic manifold geometry.
- Existing methods, assuming knowledge of manifold geometry, are impractical with sparse data.

Goal

- **Goal: Present a new method to construct intrinsic gaussian processes for regression on unknown manifolds with probabilistic metrics in point cloud. (GPUM)**

- The key goals include overcoming limitations of Euclidean Gaussian Processes, leveraging B-GPLVM and Riemannian geometry for probabilistic mapping, and defining adaptive boundaries based on uncertainty. The primary aim is to offer an effective solution for accurate manifold regression.

Method - Riemannian Metric tensor

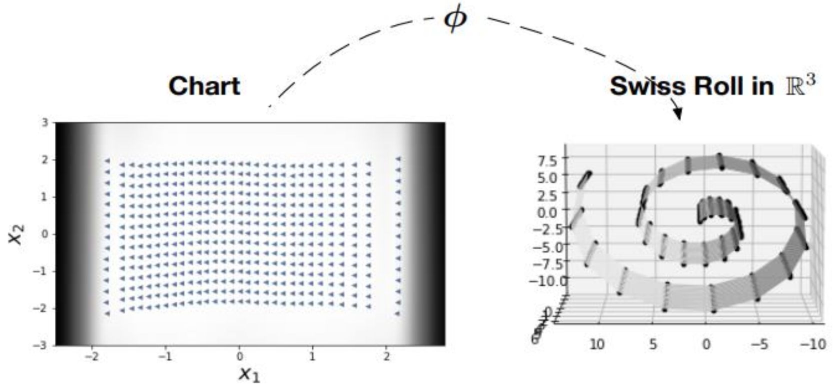
The Riemannian metric is used as a key component in understanding and characterizing the geometry of the unknown manifolds. The specific use of the Riemannian metric contributes to the probabilistic representation of manifold geometry.

- Let J denote the Jacobian of ϕ. We have: $\mathbf{g} = \mathcal{J}^T \mathcal{J}, \quad \mathcal{J}_{i,j} = \frac{\partial \phi^i}{\partial x^j}.$
- The resulting metric g follows a non-central Wishart distribution: $\mathbf{g} \sim \mathcal{W}_q\left(p, \Sigma_{\mathbf{J}}, \mathbb{E}(\mathbf{J}^T)\mathbb{E}(\mathbf{J})\right).$
- The expected metric tensor can be computed as: $\mathcal{G} = \mathbb{E}(\mathbf{g}) = \mathbb{E}(\mathbf{J}^T)\mathbb{E}(\mathbf{J}) + p\Sigma_{\mathbf{J}}$
- The boundary of the learned manifold can be defined by: $\partial\mathbb{M} = \{x \in \mathbb{R}^q \mid \mathbb{V}ar(\phi(x)|x) = \alpha\}.$

Method-Latent Space

The latent space, introduced through B-GPLVM, serves as a crucial component in GPUM, enabling probabilistic mapping, learning metric tensor distribution, uncertainty quantification, adaptive boundary definition, and dynamic insights into manifold dynamics.

- A manifold embedded in a high dimensional Euclidean space can be well described by a probabilistic mapping function φ and the corresponding latent space. The mapping function could be GPLVM Model etc.



$$s_i^j = \phi^j(x_i) + e_i^j,$$

Method-Heat Kernel and Brownian Motion

The heat kernel is estimated as the transition density of Brownian Motıon and used as the covariance functions of GPUM .

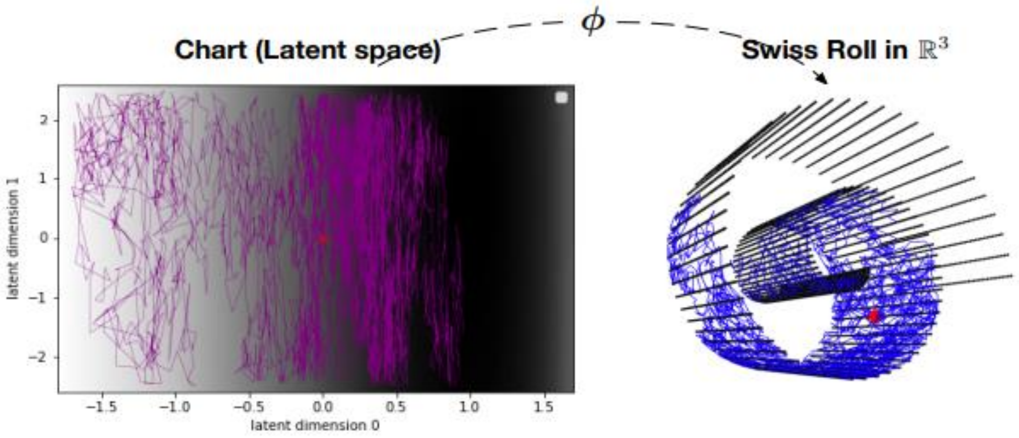
- If M is a Euclidean space R^q , the heat kernel has a closed form corresponding to a time-varying Gaussian function, Consider the heat equation on M, given by:

$$\frac{\partial}{\partial t} K_{heat}(s_0, s, t) = \frac{1}{2} \Delta_s K_{heat}(s_0, s, t), \qquad s_0, s \in \mathbb{M},$$

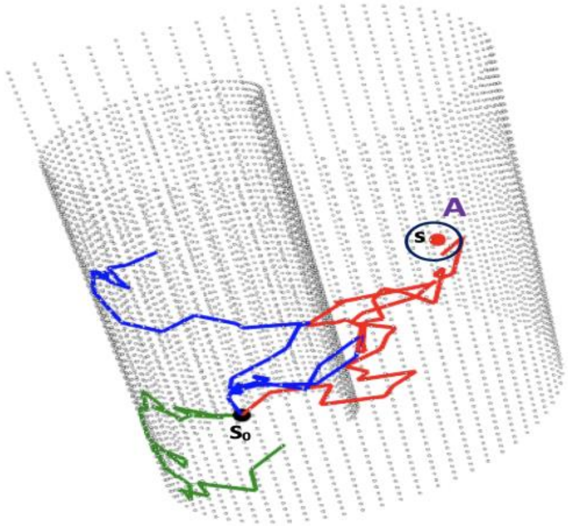
- **We estimated the heat kernel as the BM transition density (Hsu,1988) by simulating Brownian Motion paths.** The BM on a Riemannian manifold in a local coordinate system is given as a system of stochastic differential equations in the Itˆo form:

$$dx^i(t) = \frac{1}{2} G^{-1/2} \sum_{j=1}^{q} \frac{\partial}{\partial x^j} \left(\mathcal{G}^{ij} G^{1/2} \right) dt + \left(\mathcal{G}^{-1/2} dB(t) \right)_i$$

Method-Brownian Motion and Transition Density



- A BM sample path (blue line, right panel) on M (Swiss roll in R^3) and its equivalent stochastic process (purple line, left panel) in the chart (or latent space) in R^2 . ϕ : R^2 → M ⊂ R^3 is a parametrization of M.



$$K_{heat}^{t}(s_0, s) \approx \frac{p(\mathbf{S}(t) \in \mathbf{A}_s \mid \mathbf{S}(0) = s_0)}{V(\mathbf{A}_s)} \approx \frac{1}{V(\mathbf{A}_s)} \cdot \frac{N_{A_s}}{N_{BM}} = \hat{K}_{heat}^{t}$$

Method-GPLVM and Bayesian GPLVM

They provide a way to map high-dimensional data to a lower-dimensional latent space using Gaussian processes.

- GPLVM: The probability of the observed data

$$p(\mathcal{S}, \Phi | \mathcal{X}, \beta) = p(\mathcal{S} | \Phi, \beta) p(\Phi | \mathcal{X}) = \prod_{j=1}^{p} p(\mathbf{s}_{:}^{j} | \boldsymbol{\phi}_{:}^{j}, \beta) p(\boldsymbol{\phi}_{:}^{j} | \mathcal{X}),$$

For a point x_∗ in the latent space, the distribution of the Jacobian takes the form

$$\begin{aligned} p(\mathbf{J} | \mathcal{X}, \mathcal{S}) &= \prod_{j=1}^{p} \mathcal{N}(\mu_{\mathbf{J}}^{j}, \Sigma_{\mathbf{J}}) \\ &= \prod_{j=1}^{p} \mathcal{N}(\partial K_{\mathcal{X},*}^{T} K_{\mathcal{X},\mathcal{X}}^{-1} \mathbf{s}_{:}^{j}\ , \partial^{2} K_{*,*} - \partial K_{\mathcal{X},*}^{T} K_{\mathcal{X},\mathcal{X}}^{-1} \partial K_{\mathcal{X},*}). \end{aligned}$$

- Bayesian Gaussian Processes Latent Variable Models (B-GPLVM) go beyond GPLVM by introducing a Bayesian framework.

Compared Method-Graph Laplacian

Graph Laplacian is a mathematical construct associated with a graph, a structure composed of nodes (or vertices) and edges connecting pairs of nodes.

Algorithm 2: GL Algorithm.

Algorithm inputs include t, ϵ, K

Step (1): Construct the $(n+v) \times (n+v)$ matrix W and D as shown in Appendix I with bandwidth ϵ and points cloud $\{x_1, \ldots, x_{n+v}\}$. We can get:

$$\tilde{A} = D^{-1/2} W D^{-1/2}.$$

Step (2): Find the first $K-1$ eigenpairs of $\tilde{A}$:

$$\{\alpha_{i,\epsilon}, U_{i,\epsilon}\}_{i=1}^{K-1}.$$

Step (3): Suppose $\tilde{v}_{i,\epsilon}$ is the normalized vector of $D^{-1/2}U_{i,\epsilon}$ in the l^2 norm, and we have:

$$\mu_{i,\epsilon} := \frac{1-\alpha_{i,\epsilon}}{\epsilon^2}.$$

Let $N(i) = |B_\epsilon^{R^p}(f(x_i))\{f(x_1)\ldots f(x_n)\}|$ be the number of points on ϵ ball in the ambient space,We have the l^2 norm of $\tilde{v}$:

$$\tilde{v}_{l^2} = \sqrt{\frac{|S^{d-1}|\epsilon^d}{d}\sum_{i=1}^{n}\frac{\tilde{v}^2(i)}{N(i)}}.$$

For $i = 1, 2, \ldots, K-1$, we have: $v_{i,\epsilon} = \frac{\tilde{v}_{i,\epsilon}}{\tilde{v}_{l^2}}$

Construct $H_{\epsilon,t}^K$ as

$$H_{\epsilon,t}^K = \sum_{i=0}^{K-1} e^{-\mu_{i,\epsilon}} v_{i,\epsilon} v_{i,\epsilon}^T.$$

Result-Swiss Roll

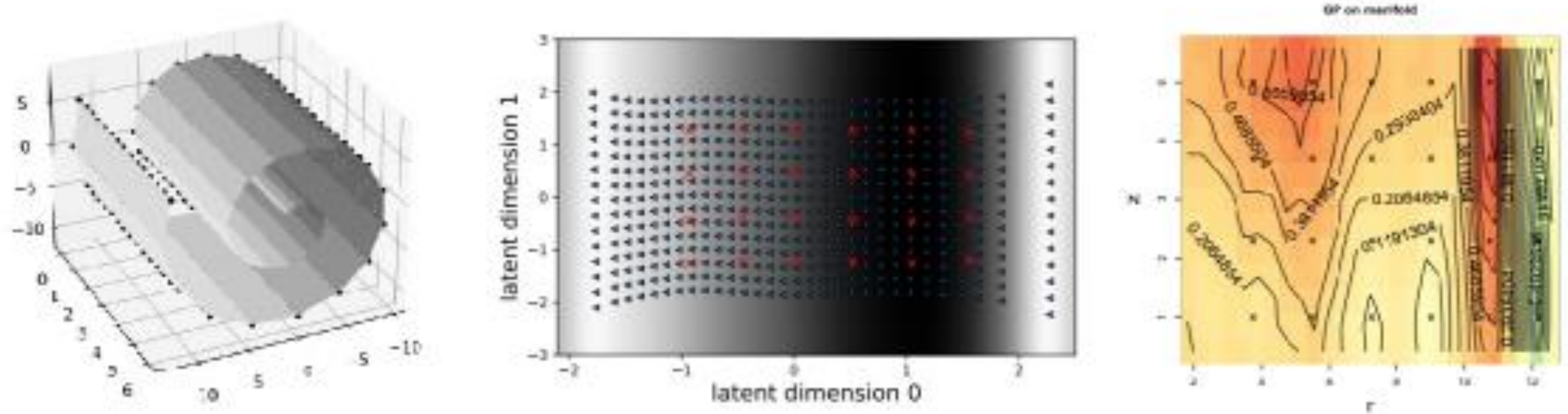
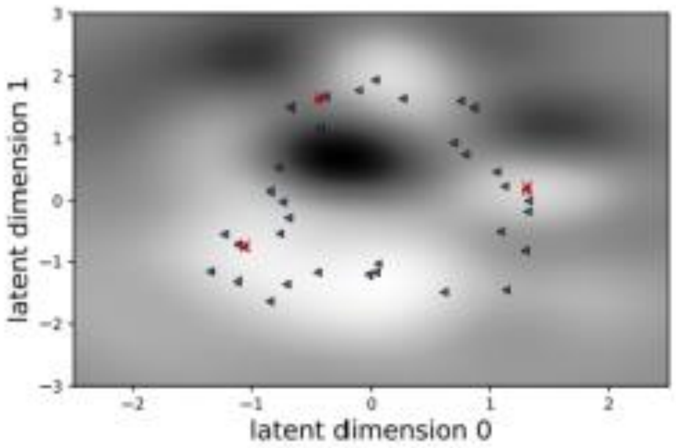
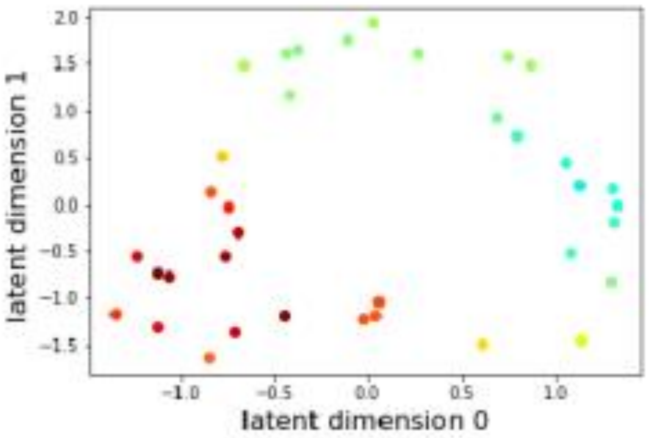


Figure 2: Swiss roll point cloud in ^{3} (left); Latent space and magnification factor(middle); GPUM prediction(right)

	$\mathbb{R}^3GP$	$\mathbb{R}^2GP$	GPUM	GL-GP	GM-GP
RMSE $v = 250$	0.284(0.006)	0.293(0.005)	0.163(0.020)	0.243(0.003)	0.231(0.001)
RMSE $v = 450$	0.298(0.007)	0.290(0.005)	0.162(0.003)	0.220(0.002)	0.207(0.002)
RMSE $v = 800$	0.287(0.006)	0.282(0.005)	0.164(0.002)	0.216(0.001)	0.206(0.001)

Result- Wifi Signal





	$\mathbb{R}^{30}$GP	$\mathbb{R}^{2}$GP	GPUM	GL-GP	GM-GP
MEAN RMSE	5.57(1.43)	4.83(1.83)	4.11(0.88)	5.6(1.15)	6.04 (0.57)

Result- Camera angle estimation from images.

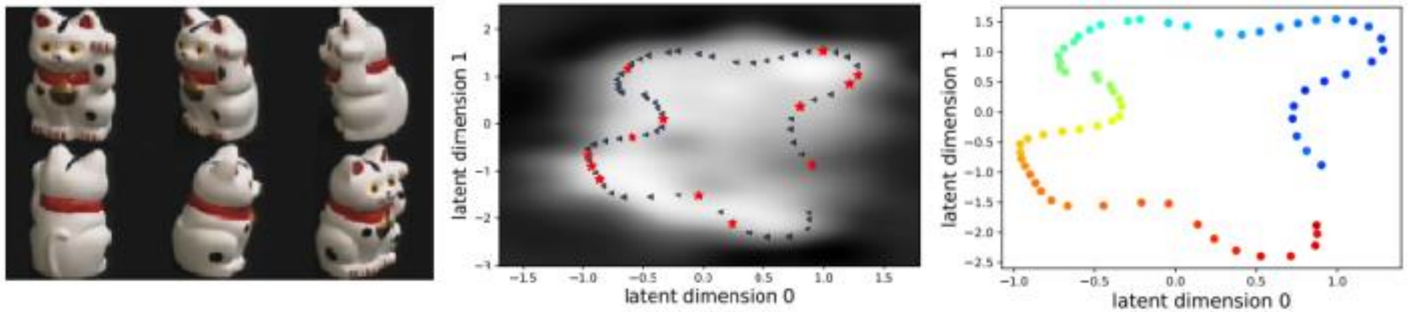


Figure 4: Coil images (left); Latent space and magnification factor (middle); GPUM prediction(right)

	$\mathbb{R}^{1024}$GP	$\mathbb{R}^{2}$GP	GPUM	GL-GP	GM-GP
MEAN RMSE	0.097(0.040)	0.094(0.042)	0.060(0.038)	0.116(0.027)	0.143(0.026)

Conclusion

1. Introduces a new framework for regression on high-dimensional point cloud implicit manifolds: GPUM, using probabilistic latent variable models to learn the geometry of implicit manifolds and provide local metric distributions.
2. BM simulations using the B-GPLVM metric yield similar results to those using the analytical metric.
3. GPUM is constructed based on the equivalence relationship between heat kernels and BM transition density on manifolds, allowing it to incorporate the intrinsic geometry of the implicit manifold for inference while respecting internal constraints and boundaries.

Thank you for listening

#UofGWorldChangers

@UofGlasgow