Wrapped Gaussian Process Regression on Riemannian Manifolds

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Summary

- Gaussian process (GP) regression is a powerful tool in non-parametric regression providing uncertainty estimates. However, it is limited to data in vector spaces, thus not suitable for non-linear geometries (see Fig. 1).
- We tackle this problem by defining wrapped Gaussian processes (WGPS) on Riemannian manifolds, using the probabilistic setting to generalize GP regression to the context of manifold-valued targets.
- We experiment on diffusion weighted imaging (DWI) data, experimental on diffusion weighted imaging (DWI) data, and flexible tool for manifold-valued regression.

Wrapped Gaussian Processes

- A collection f of random points on a manifold M indexed over a set Ω is a wrapped Gaussian process (WGP), if every finite subcollection \((f(\omega_1), ..., f(\omega_n))\) \(\omega_i \in \Omega\), is jointly WGD on \(M^N\). We define

\[
X = \text{Exp}_p(Y),
\]

then \(X\) has a wrapped Gaussian distribution, denoted by \(X \sim \mathcal{N}_M(p, k)\). Furthermore, we define the maps \(\mu_{\mathcal{N}_M}(X) := \mu\) and \(\text{Cov}_{\mathcal{N}_M}(X) := K\), as shown in Fig. 2 a).

- The random points \(X_1, X_2 \sim \mathcal{N}_M(p_i, k_i), i = 1, 2\), are jointly WGD, if the random point \((X_1, X_2)\) on \(M_1 \times M_2\) is WGD, that is,

\[
(X_1, X_2) \sim \mathcal{N}_M(p_1, k_1 \times p_2, k_2),
\]

for some matrices \(K_{12} = K_{12}^T\).

Theorem 1 Assume \(X_1, X_2\) are jointly WGD as in (2), then we have the conditional distribution

\[
X_1|X_2 = x_2 \sim \mathcal{N}(\mu, K_2) = \left(\begin{array}{c}
\mu
\
K_2
\end{array}\right)
\]

where

\[
\mu = \mu_1 - K_{12} K_2^{-1} x_2
\]

\[
K = K_1 - K_{12} K_2^{-1} K_{12}^T
\]

\[
\lambda_{v} = \frac{1}{\text{Tr}(K_0)}
\]

\[
A = \{v \in T_v M | \text{Exp}_v(p_2) = p_1\}
\]

\[
P'(A) = \int_{A} \frac{1}{\text{det}(\lambda_{v})} \text{Exp}_v(p_2) dv
\]

and \(f(A) = \mu(f^{-1}(A))\) for measure \(\mu\) and measurable \(f, A\).

Wrapped Gaussian Processes

- A collection \(f\) of random points on a manifold \(M\) indexed over a set \(\Omega\) is a wrapped Gaussian process (WGP), if every finite subcollection \((f(\omega_1), ..., f(\omega_n))\) \(\omega_i \in \Omega\), is jointly WGD on \(M^N\). We define

\[
m(\omega) := \mu_{\mathcal{N}_M}(f(\omega))
\]

\[
k(x, \omega) := \text{Cov}_{\mathcal{N}_M}(f(x), f(\omega))
\]

called the basepoint function and tangent space covariance function of \(f\). See Fig. 2 b) for a visualization.

WGP Regression

- The learning goal is as follows: given data \(D_M = \{(x_i, p_i)\}_{i=1}^m\) and assuming \(p_i = f(x_i)\) for some map \(f : \mathbb{R}^d \rightarrow M\), infer \(f\).

- Approach: define a prior distribution \(f \sim \mathcal{GP}(m, k)\) and condition on the data given the using Theorem 1. The process is given in Algorithm 1 and illustrated in Fig. 3.

Algorithm 1: WGP Regression

Data: \(D_M = \{(x_i, p_i)\}_{i=1}^m\).

Result: Predictive distribution for \(p_i\) at \(x_i\).

i. Choose a prior basepoint function \(m\).

ii. Transform \(D_M \leftarrow \{(x_i, \text{Log}_m(p_i))\}_{i=1}^m\).

iii. Choose a prior tangent space covariance function \(k\) from a parametric family by optimizing the hyperparameters.

iv. Using GP prior \(\mathcal{GP}(m, k)\), carry out Euclidean GP regression for the transformed data \(D_M\), yielding the mean and covariance \((\mu, \Sigma)\).

v. End with the predictive distribution \(p_i \sim \mathcal{GP}(\mu, \Sigma)\).

Experiments

- We demonstrate WGP regression on three different manifolds; the 2-sphere, the space of 3-by-3 covariance matrices, and the Kendall shape space.

- In the sphere experiment, we use the RBF and periodic covariance functions (kernels). For the rest, we use the RBF kernel with hyperparameters chosen to maximize the likelihood of observed data.

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