Data-driven Warping of Gaussian Processes for Spatial Interpolation of Skewed Data

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Motivation

- Generating accurate estimates and maps from sparse, non-Gaussian data remains a challenge.
- Observed data distributions do not always comply with explicit mathematical models.
- Machine learning is in fashion; how does geostatistics fit in?



What are Gaussian Process Regression (GPR) and Data-driven Warping?

- Gaussian processes are Gaussian random fields defined in feature spaces.
- GPR prediction is "equivalent" to kriging in feature space.
- "Warping" the process means applying a nonlinear transform to normalize the data before the regression step [Snelson et al., 2004].
- Data-driven warping means that the warping transform is learned from the data using a non-parametric, kernel-based estimator.

(1) Agou, Pavlides, Hristopulos. "Spatial Modeling of Precipitation Based on Data-Driven Warping of Gaussian Processes." *Entropy* 2022, 24, 321.

(2) Pavlides, Agou, Hristopulos. "Non-parametric Kernel-Based Estimation of Probability Distributions for Precipitation Modeling." *arXiv preprint*, arXiv:2109.09961 (2021).

Learning the Cumulative Distribution Function using Kernels

- Kernel functions are used to estimate the CDF.
- CDF steps are smoother than the staircase estimate.
- A theoretical model of the probability distribution is not necessary.



Warped Gaussian Process Regression in a Nutshell



Gaussian Process Regression (GPR) compared to wGPR for Test Function

$$egin{aligned} x(m{s}) &= \left[\sin(\pim{s}) + \sigma_\epsilon\,\epsilon(m{s})
ight]^{1/3}, \quad m{s} \in [-1,1] \ \sigma_\epsilon &= 0.1, \; \epsilon(m{s}) \sim \mathcal{N}(0,1) \end{aligned}$$



Example: SIC 1997 Swiss Rainfall Data



Training: 100 points. Validation: 367 points. Map Grid: 6251 point inside convex hull. Optimal variogram: Spartan variogram (Boltzmann-Gibbs with gradient and curvature terms). Kernel for warping: Epanechnikov.

Contributions

- We introduce data-driven warping which is a flexible, non-parametric approach for normalizing non-Gaussian data.
- Our approach differs from others because the normalizing transform is expressed in terms of kernel functions and the data values.
- In data-driven wGPR we combined data-driven warping with Gaussian process regression, leading to a more flexible spatial prediction method than GPR.
- wGPR allows us to use commonly known geostatistical methods in the broader framework of Gaussian processes.

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