geospaNN: A Python package for geospatial neural networks

Summary

Geostatistical models are widely used to analyse datasets with spatial information encountered frequently in the geosciences (climate, ecology, forestry, environmental sciences, and other research fields). In geostatistics, the spatial linear mixed effects model (SPLMM)

$$Y = X\beta + \epsilon(s)$$

has long been the standard approach to model such data. SPLMM accounts for the fixed effects between observations Y and covariates X via the linear regression part, while accounting for the correlation across spatial locations s via the spatial error process $\epsilon(s)$. Typically, the spatial dependency embedded in $\epsilon(s)$ is modeled using a Gaussian Process, which provides a parsimonious and flexible solution to modeling spatial correlations and provide spatial predictions at new locations via kriging.

The linear regression part of SPLMM is restrictive. Recently, machine learning techniques like artificial neural networks have been increasingly incorporated into geostatistics to address complex and non-linear interactions among variables. However, few methods were originally designed for dependent data structures and cannot directly encode correlation. Even those modified to account for spatial dependencies, like adding a large number of spatial features as inputs to neural network, still face scalability limitations due to the expanded dimensionality from adding many features. To address these concerns, we introduce `geospaNN`, a Python software for analysis of geospatial data using neural networks. `geospaNN` implements NN-GLS, a novel adaptation of Neural Networks (NN) proposed in Zhan and Datta (2024). NN-GLS bridges ideas of geostatistical modeling and machine learning by embedding neural network with spatial mixed models, retaining the capacity to directly model spatial correlations. NN-GLS extends the SPLMM to non-linear scenarios by replacing $X\beta$ with $m(X)$, a non-linear function. NN-GLS simultaneously performs non-linear mean function estimation using a neural network and spatial predictions (including prediction intervals) using Gaussian processes. For computational efficiency, `geospaNN` leverages the widely popular Nearest Neighbor Gaussian Process (NNGP) approximation Finley et al. (2019). It is also, to our knowledge, the first Python package to implement NNGP for scalable covariance matrix computations in geostatistical mmodels. This is a standalone component of broad and independent utility.

Statement of Need

`geospaNN` is a Python package for geospatial analysis that uses NN-GLS, a novel and scalable class of neural networks explicitly designed to account for spatial correlation in the data. The package implements NN-GLS using PyTorch, an open-source library widely used for building machine learning models. As illustrated in Zhan and Datta (2024), `geospaNN` is effectively represented as a geographically-informed Graph Neural Network (GNN) by using NNGP covariance matrices. It can be embedded within the PyG (PyTorch Geometric) framework, which is designed for scalable execution of GNNs on irregular data structures like graphs. `geospaNN` is primarily intended for researchers and scientists in machine learning and spatial statistics, but can also be applied more generally to estimation and prediction tasks involving other data with dependency structures, like time-series. `geospaNN` provides user-friendly wrappers for data simulation, preprocessing, and model training, which significantly simplify the analytical pipeline.

The implementation of NNGP models within `geospaNN` is of independent importance. NNGP enables scalable covariance matrix inversions, which features extensively in geospatial models. There exist two widely used R-packages `spNNGP` (Finley et al. 2019) and `BRISC` (Saha and Datta 2018) for implementations of NNGP, but to our knowledge there is no Python implementation of NNGP. We thus offer an avenue to efficiently analyze massive geospatial datasets in Python using NNGP (linear models) and NN-GLS (non-linear models).

The goal of `geospaNN` is to provide a lightweight, efficient, and user-friendly machine learning tool for geospatial analysis that can directly model spatial correlation. According to simulations, the package can handle datasets with up to half a million observations in under an hour on a standard personal laptop (Macbook with an M1 8-core processor, 16 GB Unified RAM). A significant portion of `geospaNN` has already been used in articles such as Zhan and Datta (2024) and Heaton, Millane, and Rhodes (2024). In the future, we anticipate that `geospaNN` will play a significant role at the interface of machine learning and spatial statistics, serving as a foundation for both scientific and methodological explorations.

State of the field

In Python, geospatial data is primarily processed using the `GeoPandas` library (Jordahl et al. 2021), which enables efficient spatial operations and visualization. Meanwhile, deep learning frameworks such as `PyTorch` (Paszke et al. 2019) are widely used for advanced machine learning applications. To integrate geospatial data with deep learning, several specialized tools have been developed. Notably, `TorchGeo` (Stewart et al. 2022) extends `PyTorch` for tasks such as land cover classification, object detection, and geospatial segmentation. Independently, the R package `geodl` (Maxwell et al. 2024) was recently introduced for analyzing geospatial and spatiotemporal data. Implemented in R (`terra`) and C++, `geodl` operates without requiring a Python environment. However, these tools have certain limitations. For example, `TorchGeo` primarily supports raster and vector data, such as satellite imagery, while `geodl` is designed for pixel-level applications (e.g., semantic segmentation) and requires data transformation into a raster-based format.

Integrating spatial information from data collected at an irregular set of locations into a graph enhances the flexibility and effectiveness of geospatial analysis. One of the most widely used approaches for data with irregular geometry is Graph Neural Network (GNN), which efficiently processes graph-structured data by learning node, edge, and graph-level representations through message passing and aggregation. For GNN implementation, the PyTorch Geometric (PyG) library, built on PyTorch, provides a highly customizable framework for defining graph convolutional layers (Fey and Lenssen 2019). GNNs have been widely applied in geospatial analysis, with notable examples including disease forecasting (Tonks et al. 2024), crop yield prediction (Fan et al. 2022), and traffic flow modeling (Wang et al. 2020). However, despite their growing adoption, there is still no systematic analytical software tailored for broad use within the statistical community.

The geospaNN Package

This section provides an overview of the `geospaNN` package, including the NN-GLS architecture and several technical details. For practical examples and detailed documentation, visit the `geospaNN` website at https://wentaozhan1998.github.io/geospaNN-doc. A vignette is also available on the website https://github.com/WentaoZhan1998/geospaNN/blob/main/vignette/vignette.pdf for detailed illustration of various usage of the package.

NN-GLS Overview

In a simple linear regression scenario, Gauss-Markov's Theorem states that when the data exhibits a correlation structure, generalized least squares (GLS) provides greater efficiency than ordinary least squares (OLS).

For vanilla neural networks, it is typically implicitly assumed that the observations Y_i are not correlated, and mean squared error is used as the loss function for regression tasks for continuous outcomes:

$$Y = m(X) + \epsilon.$$

NNGLS considers a similar model for spatial data:

$$Y(s) = m(X(s)) + \epsilon(s)$$

where $Y(s)$ and $X(s)$ are respectively the outcome and covariates observed at location s, m is a non-linear function relating $X(s)$ to $Y(s)$, to be estimated using a neural network. The key distinction from the standard non-linear regression setup is that here the errors $\epsilon(s)$ is a dependent process that models spatial correlation. Typically it is decomposed as the sum of a Gaussian process for the spatial dependence and, possibly, a noise component. Given the observations Y, the covariates X, and the locations s as the input, NN-GLS estimates the mean function $m()$ and predicts Y at new locations. The ultimate goal of NN-GLS is to help understanding the complex relationship between observations and covariates and provide accurate geospatial prediction.

Let Σ be a model for the spatial error ϵ, then the well-known theory (Gauss-Markov theorem) of OLS and GLS from the statistical literature motivates the introduction of a GLS-style loss in neural networks:

$$L\big(m(\cdot)\big) = \frac{1}{n}\big(Y - m(X)\big)^\top \Sigma^{-1}\big(Y - m(X)\big).$$

However, minimizing this GLS-style loss in practice presents several challenges:

1. The covariance matrix Σ is based on a parametric covariance function, and the parameters are typically unknown.
2. Even if Σ is well-estimated, inverting Σ becomes computationally infeasible as the sample size n grows large.
3. Since the GLS loss is not additive across observations, mini-batching—an essential technique used in implementation of modern neural networks—cannot be applied directly.

NN-GLS addresses these issues by introducing the Nearest Neighbor Gaussian Process (NNGP) to approximate Σ^{-1}, and it naturally equates to a specialized Graph Neural Network (GNN). In brief, NNGP is a nearest-neighbor-based approximation to a full Gaussian Process with a specific covariance structure (Datta 2022). On a finite sample, NNGP sparsifies the covariance matrix, thus simplifying both likelihood computation and the GLS-style loss, addressing the three issues mentioned above.

Specifically, for the GLS loss function:

$$L\big(m(\cdot)\big) = \frac{1}{n}\big(Y - m(X)\big)^\top \Sigma^{-1}\big(Y - m(X)\big) = \frac{1}{n}\big(Y^* - m^*(X)\big)^\top \big(Y^* - m^*(X)\big) = \frac{1}{n}\sum_{i=1}^{n}(Y_i^* - m^*(X_i))^2,$$

where $Y^* = Q^{1/2}Y$ and $m^*(X) = Q^{1/2}m(X)$ can be obtained easily using aggregation over the nearest-neighbot directed acyclic graph specifying the NNGP approximation. The GLS loss returns to an additive form, allowing for mini-batching instead of full-batch training. For likelihood-based parameter estimation, `geospaNN` uses the `BRISC` R package as an efficient solution (Saha and Datta 2018).

In NN-GLS, we assume that the parameters of the covariance matrix is unknown. The spatial parameters θ and the weights and biases parameters of the neural network used to model m are estimated iteratively, and training proceeds until the validation loss converges. Once estimation is complete, nearest-neighbor-based kriging is used to generate spatial predictions and prediction intervals at new locations. The whole procedure embeds the three core features of `geospaNN`,

1. estimate the non-linear mean function by $\hat{m}$.
2. estimate the spatial parameters by $\hat{\theta}$.
3. predict the outcome at new locations by $\hat{Y}$.

NNGP and Other Features

In addition to estimation and prediction for the non-linear spatial mixed model using NN-GLS, `geospaNN` offers a standalone efficient implementation of the spatial linear mixed model using NNGP. Given an $n \times n$ covariance matrix Σ and a k-neighbor list (defaulting to nearest neighbors), our implementation guarantees $O(n)$ computational complexity for any approximate matrix products involving $\Sigma^{1/2}$, $\Sigma^{-1/2}$, and Σ^{-1}. The option of customizing the k-neighbor list is provided in case specially designed neighbor set is desired, like using distant neighbors to model long-range correlation (Stein, Chi, and Welty 2004), or neighbors based on geodesic-distances if working with data collected on a non-Euclidean domain like water bodies (Gilbert and Datta 2024). NNGP is fundamental to several key scalable features in `geospaNN`, including spatial data simulation and kriging.

For simulation, `geospaNN` allow users to customize the spatial parameters and mean functions to generate Y, X, and s from the spatial non-linear mixed model. Users are allowed to customize the spatial coordinates to simulate under different context. This feature can be flexibly used to simulate a Gaussian process as a general spatial random effect by specifying a zero mean function. For kriging, instead of using the full observed set, only the nearest neighbors of each new spot in the observed set are used to compute the kriging weights. It has been shown in Zhan and Datta (2024) that the nearest neighbor kriging provide accurate prediction interval under various settings.

`geospaNN` offers user-friendly modules for essential machine learning tasks, including neural network (NN) architecture design, training log management, and result visualization. In addition to tracking validation loss, the training log also visualizes the evolution of spatial parameters, providing deeper insight into model convergence. For high-dimensional result interpretation, `geospaNN` incorporates partial dependence plots (PDPs) to illustrate the marginal effect of individual covariates on the outcome. When compared across multiple models, PDPs offer invaluable insights into the complex relationships between covariates and the predicted outcome.

As a special case of the spatial non-linear mixed model, SPLMM with NNGP covariance is also implemented in `geospaNN`. The implementation here is equivalent to the R-package `BRISC` and should be an optimal choice for the Python users if efficient SPLMM solution is wanted for large geospatial datasets.

All these functions are included explicitly in the package and can be called independently.

Discussion

The `geospaNN` package offers an efficient implementation of the geospatial neural networks, specifically, the NN-GLS approach proposed in Zhan and Datta (2024). NN-GLS embeds a neural network with the spatial mixed model, accounts for spatial correlation by replacing the original loss function with a GLS-style version. `geospaNN` is capable of performing various statistical tasks, including non-linear mean-function estimation, covariance parameter estimation, spatial prediction with uncertainty quantification. The NNGP approximation, which is fundamental to the scalable implementation of `geospaNN`, is offered as a standalone functionaility in `geospaNN`. This to our knowledge is the only Python implementation of the widely popular NNGP model for scalable geostatistical analysis. Moreover, due to the sparsity of the NNGP approximation, `geospaNN` can be seamlessly integrated into the framework of Graph Neural Networks (GNNs), opening up new possibilities for a wide range of advanced neural architectures. A promising future direction for `geospaNN` is to evolve into a general framework for geospatially-informed deep learning, where graph-based message-passing (convolution) can occur multiple times, with weights determined by spatial processes to maintain statistical interpretability. We are also planning to explore the extension of `geospaNN` towards other data types and distributions in the future.

Acknowledgements

References

Datta, Abhirup. 2022. "Nearest-Neighbor Sparse Cholesky Matrices in Spatial Statistics." *Wiley Interdisciplinary Reviews: Computational Statistics* 14 (5): e1574.

Datta, Abhirup, Sudipto Banerjee, Andrew O Finley, and Alan E Gelfand. 2016. "On Nearest-Neighbor Gaussian Process Models for Massive Spatial Data." *Wiley Interdisciplinary Reviews: Computational Statistics* 8 (5): 162–71.

Fan, Joshua, Junwen Bai, Zhiyun Li, Ariel Ortiz-Bobea, and Carla P Gomes. 2022. "A GNN-RNN Approach for Harnessing Geospatial and Temporal Information: Application to Crop Yield Prediction." In *Proceedings of the AAAI Conference on Artificial Intelligence*, 36:11873–81. 11.

Fey, Matthias, and Jan E. Lenssen. 2019. "Fast Graph Representation Learning with PyTorch Geometric." *arXiv Preprint arXiv:1903.02428*.

Finley, Andrew O, Abhirup Datta, Bruce D Cook, Douglas C Morton, Hans E Andersen, and Sudipto Banerjee. 2019. "Efficient Algorithms for Bayesian Nearest Neighbor Gaussian Processes." *Journal of Computational and Graphical Statistics* 28 (2): 401–14.

Gilbert, Brian, and Abhirup Datta. 2024. "Visibility Graph-Based Covariance Functions for Scalable Spatial Analysis in Non-Convex Partially Euclidean Domains." *Biometrics* 80 (3): ujae089.

Heaton, Matthew J, Andrew Millane, and Jake S Rhodes. 2024. "Adjusting for Spatial Correlation in Machine and Deep Learning." *arXiv Preprint arXiv:2410.04312*.

Jordahl, Kelsey, Joris Van den Bossche, Jacob Wasserman, James McBride, Jeffrey Gerard, Jeff Tratner, Matthew Perry, and Carson Farmer. 2021. "Geopandas/Geopandas: V0. 5.0." *Zenodo*.

Maxwell, Aaron E, Sarah Farhadpour, Srinjoy Das, and Yalin Yang. 2024. "Geodl: An r Package for Geospatial Deep Learning Semantic Segmentation Using Torch and Terra." *PloS One* 19 (12): e0315127.

Paszke, Adam, Sam Gross, Francisco Massa, Adam Lerer, James Bradbury, Gregory Chanan, Trevor Killeen, et al. 2019. "Pytorch: An Imperative Style, High-Performance Deep Learning Library." *Advances in Neural Information Processing Systems* 32.

Saha, Arkajyoti, and Abhirup Datta. 2018. "BRISC: Bootstrap for Rapid Inference on Spatial Covariances." *Stat* 7 (1): e184.

Stein, Michael L, Zhiyi Chi, and Leah J Welty. 2004. "Approximating Likelihoods for Large Spatial Data Sets." *Journal of the Royal Statistical Society Series B: Statistical Methodology* 66 (2): 275–96.

Stewart, Adam J., Caleb Robinson, Isaac A. Corley, Anthony Ortiz, Juan M. Lavista Ferres, and Arindam Banerjee. 2022. "TorchGeo: Deep Learning with Geospatial Data." In *Proceedings of the 30th International Conference on Advances in Geographic Information Systems*, 1–12. SIGSPATIAL '22. Seattle, Washington: Association for Computing Machinery. https://doi.org/10.1145/3557915.3560953.

Tonks, Adam, Trevor Harris, Bo Li, William Brown, and Rebecca Smith. 2024. "Forecasting West Nile Virus with Graph Neural Networks: Harnessing Spatial Dependence in Irregularly Sampled Geospatial Data." *GeoHealth* 8 (7): e2023GH000784.

Wang, Xiaoyang, Yao Ma, Yiqi Wang, Wei Jin, Xin Wang, Jiliang Tang, Caiyan Jia, and Jian Yu. 2020. "Traffic Flow Prediction via Spatial Temporal Graph Neural Network." In *Proceedings of the Web Conference 2020*, 1082–92.

Zhan, Wentao, and Abhirup Datta. 2024. "Neural Networks for Geospatial Data." *Journal of the American Statistical Association*, no. just-accepted: 1–21.