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A NEURAL NETWORK FRAMEWORK WITH EMBEDDED EXPERIMENTAL VARIOGRAMS FOR SPARSE SPATIAL INTERPOLATION IN GEOTECHNICAL SITE INVESTIGATION

Jiawei Xie
Discipline of Civil, Surveying and Environmental Engineering, The University of Newcastle, Callaghan, NSW 2308, Australia
E-mail: Jiawei.Xie@newcastle.edu.au

Jinsong Huang
Discipline of Civil, Surveying and Environmental Engineering, The University of Newcastle, Callaghan, NSW 2308, Australia
E-mail: Jinsong.Huang@newcastle.edu.au

Shui-Hua Jiang
School of Infrastructure Engineering, Nanchang University, Xuefu Road 999, Nanchang 330031, China
E-mail: sjiangaa@ncu.edu.cn

Variogram-based spatial correlation remains fundamental in geostatistical analysis, yet traditional approaches face persistent challenges in variogram model selection and parameter estimation. This study presents a novel neural network framework that directly incorporates experimental variograms into the learning process, eliminating the need for explicit variogram model specification. By embedding the empirical variogram structure as a spatial constraint in the neural architecture, the proposed approach preserves the interpretability of geostatistical methods while leveraging the flexibility of machine learning. The proposed method automatically captures spatial correlation patterns from data without requiring manual selection of theoretical variogram models or parameter fitting procedures. Numerical experiments demonstrate that this approach achieves comparable or superior prediction accuracy to conventional geostatistical methods across various spatial correlation structures. The framework shows particular robustness in cases where traditional variogram modeling would be challenging, such as with complex spatial patterns or limited data. The results suggest that direct integration of experimental variograms into machine learning architectures offers a promising direction for automated spatial analysis while maintaining geostatistical interpretability.

Keywords: spatial prediction, neural networks, experimental variogram, geostatistics, sparse data, spatial correlation

1. Introduction

Spatial interpolation plays a vital role in geotechnical engineering by enabling the estimation of soil properties at unsampled locations(Hu et al., 2019; Xie et al., 2022a). While Kriging has been the dominant method for this purpose, it faces several fundamental challenges, particularly in dealing with the high spatial variability of geological materials and typically sparse site investigation data(Liu et al., 2024; Phoon, 2020). One significant limitation is the requirement to select and fit theoretical variogram models to describe spatial correlation patterns(Arétouyap et al., 2016). This process not only relies heavily on limited available data but often involves subjective decisions in model selection and parameter estimation, which can significantly impact interpolation accuracy(Ching and Phoon, 2017; Xie et al., 2022b).

To address these challenges, researchers have explored various approaches. Some studies have implemented Bayesian-based methods for handling limited data(e.g., Jiang et al., 2018, 2020), while others have adopted purely data-driven approaches such as sparse Bayesian learning and neural networks with compactly supported basis functions(Ching et al., 2020, 2022). However, these solutions typically either abandon the established geostatistical framework entirely, reducing interpretability, or remain wholly within traditional methods, focusing mainly on improving parameter estimation.

Recent advances in machine learning have demonstrated the effectiveness of knowledge-informed approaches across various engineering applications(Donnelly et al., 2024; Rasht-Behesht et al., 2022; Sharma et al., 2023). Physics-informed neural networks, for instance, have successfully integrated fundamental physical laws into their architectures through specialized loss functions, reducing required training samples while ensuring physically meaningful predictions. While such approaches have been successfully applied to various aspects of geotechnical engineering, including soil mechanics and unsaturated soil behavior, the potential of embedding geostatistical principles into machine learning models remains largely unexplored.

This study proposes a novel neural network framework that directly incorporates experimental variograms into the learning process, eliminating the need for theoretical variogram model selection and parameter fitting. By embedding spatial correlation patterns through specialized loss functions, this approach preserves the interpretability of geostatistical methods while leveraging the flexibility of deep learning architectures.

2. Methodology

A fundamental concept in spatial statistics is the variogram, which quantifies the degree of spatial correlation between data points. The experimental variogram $\gamma(\boldsymbol{h})$ measures the average dissimilarity between observations separated by a distance h, expressed as

$$\gamma(\boldsymbol{h}) = 1/[2N(\boldsymbol{h})]\sum[Z(\boldsymbol{x}_i) - Z(\boldsymbol{x}_i + \boldsymbol{h})]^2 \tag{1}$$

where $N(\boldsymbol{h})$ is the number of pairs of points separated by lag $\boldsymbol{h}$; $Z(\boldsymbol{x}_i)$ is the value of the variable at the location $\boldsymbol{x}_i$; $Z(\boldsymbol{x}_i + \boldsymbol{h})$ is the value at a location separated from $\boldsymbol{x}_i$ by the lag vector $\boldsymbol{h}$. Traditional approaches require fitting theoretical models (such as exponential, spherical, or Gaussian functions) to these experimental variogram values. The parameters in the variogram modelling diagram are shown in Fig. 1.

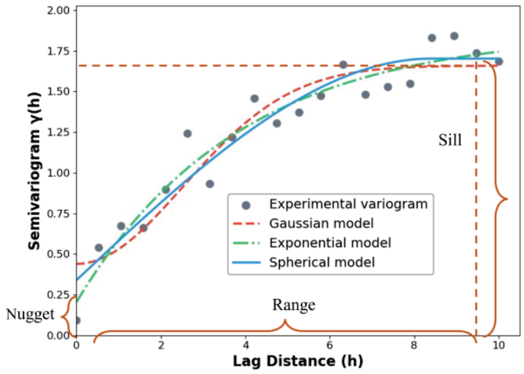

Fig. 1. Variogram modelling diagram

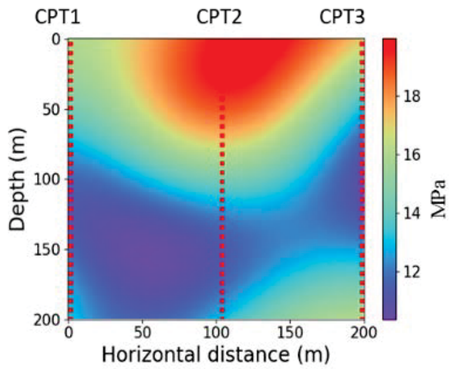

Fig. 2. Synthetic ground truth of q_t field

The mathematical relationship between covariance and variogram functions is expressed as

$$\gamma(\boldsymbol{h}) = C(0) - C(\boldsymbol{h}) \tag{2}$$

where $C(0)$ is the variance, $\boldsymbol{h}$ is the lag distance vector.

While nested variogram structures offer greater flexibility in capturing complex spatial patterns through the form $\gamma(\boldsymbol{h}) = \sum_{i=1}^{nst} C_i \Gamma_i(\boldsymbol{h})$, they introduce additional complexity in both model selection and parameter estimation.

The proposed method incorporates spatial correlation patterns directly into model training through experimental variogram constraints. The framework employs a strategic subsampling approach, selecting control points through random sampling of prediction points and inclusion of measurement locations. This ensures adequate representation of spatial patterns while maintaining computational efficiency. The variogram constraint is embedded through a dual-loss optimization structure, where the network computes the variogram loss component as

$$\text{MSE} = \frac{1}{M}\sum_h [\hat{\gamma}(h) - \gamma(h)]^2 \tag{3}$$

where M represents the number of lag distances, $\hat{\gamma}(h)$ is the variogram computed from predicted values, and $\gamma(h)$ is the experimental variogram from observed data. In this context, h represents a scalar distance.

The gradient for backpropagation follows

$$\frac{\partial \text{MSE}}{\partial \theta} = \frac{2}{M}\sum_h \frac{[\hat{\gamma}(h) - \gamma(h)]}{N(h)} \sum_{i=1}^{N(h)} [Z(x_i) - Z(x_i + h)] \left[\frac{\partial Z(x_i)}{\partial \theta} - \frac{\partial Z(x_i + h)}{\partial \theta}\right] \tag{4}$$

This formulation enables the network to learn spatial patterns directly from data without requiring explicit variogram model selection or parameter fitting. During training, we modify the loss function by incorporating the additional variogram-based MSE term from Eq. (3) into the standard prediction error. By jointly minimizing both pointwise and spatial correlation losses through backpropagation, the network learns to accurately predict values while respecting the observed variogram structure.

3. Results and discussion

To validate the proposed framework, a synthetic test case is created as shown in Fig. 2, which represents a field of cone penetration test (CPT) corrected cone tip resistance(q_t). The test domain consists of a 200×200m grid with three CPT measurement locations strategically placed at 1 m, 100 m, and 200 m along the horizontal direction. The ground truth field is generated using a Gaussian random field with a range of 100 m, mean value of 15 MPa, and variance of 8 MPa². To evaluate the framework's ability to incorporate different spatial correlation patterns, the neural network is tested using various variogram constraints by systematically varying the range values (10, 50, 100, and 150 m) while keeping the mean and variance constant. For each case, the network computed experimental variogram values using 50 equidistant lag distances between 0-120 m.

Rather than attempting to estimate the variogram structure, this study examined how well the neural network could integrate prescribed variogram models with different ranges while maintaining other parameters constant. The predicted results are provided in Fig.3.

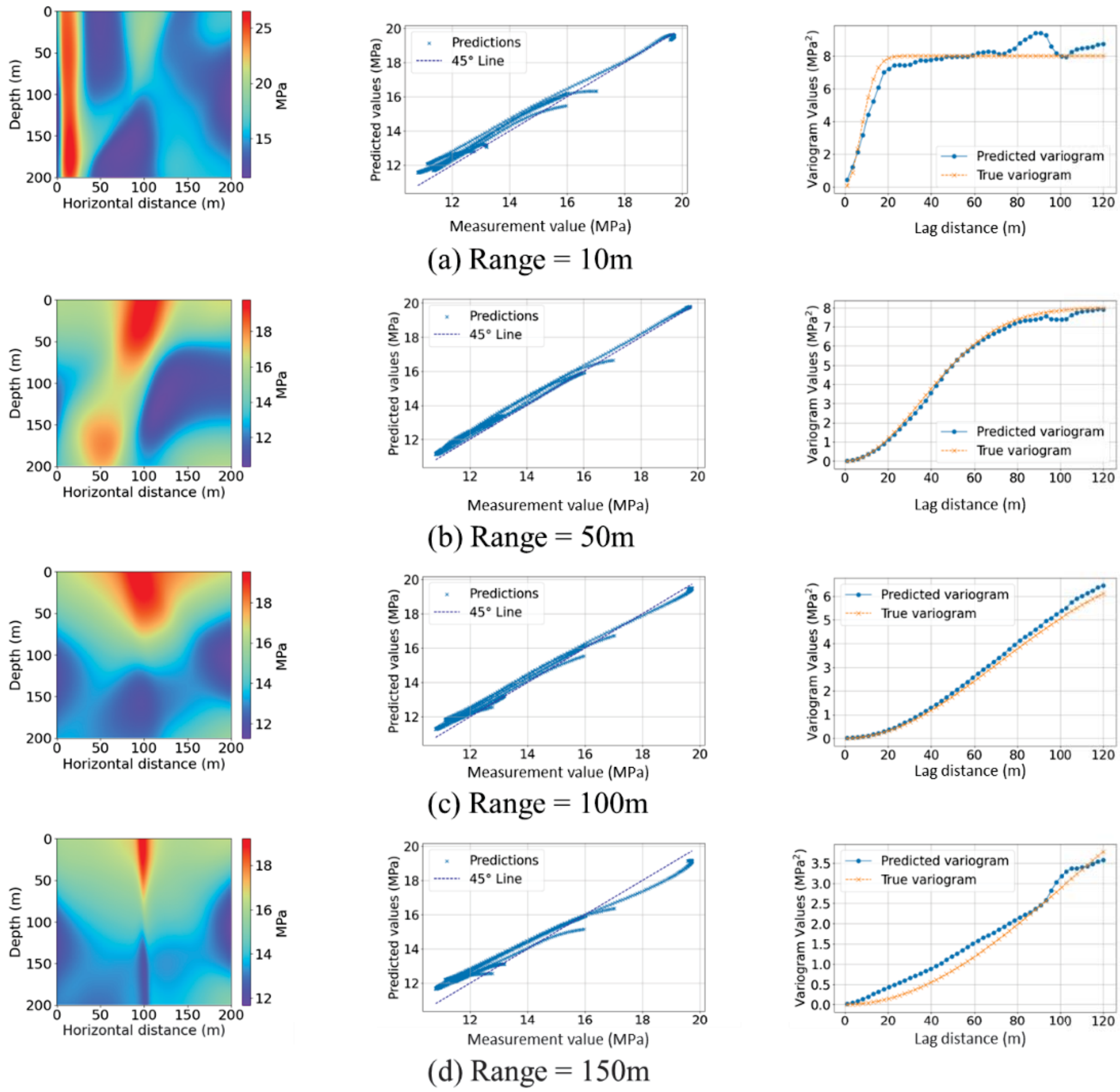

Fig. 3. Effect of using variogram loss in neural network prediction

The prediction errors show a systematic pattern: 4.62 MPa at 10m, 2.75 MPa at 50m, 1.02 MPa at 100m, and 1.62 MPa at 150m. The minimum error occurring at 100m range aligns with the ground truth's correlation structure, validating that the neural network successfully incorporated the spatial correlation constraints.

The prediction results clearly demonstrate how the neural network effectively translates the prescribed range parameters into spatially coherent predictions while maintaining high accuracy at measurement locations. At all CPT measurement points, the predicted values closely match the observed data, demonstrating the framework's ability to honor local measurements. When constrained by a smaller range (10m), the predictions exhibit rapid spatial variations and sharp transitions. As the prescribed range increases to 50m and 100m, the predicted fields show progressively smoother transitions, accurately reflecting the longer correlation lengths specified in the variogram constraints. This finding confirms that the neural network framework can successfully embed and honor different spatial correlation constraints specified through variogram models while preserving accuracy at measurement locations.

4. Conclusion

This study developed a novel neural network framework that directly incorporates experimental variograms into the learning process, eliminating the need for explicit variogram model specification in geostatistical analysis. The key findings from our numerical experiments include: (1) The proposed framework successfully generates predictions that honor both measured data points and spatial correlation patterns, effectively balancing point-wise accuracy with spatial structure constraints; (2) The prediction accuracy reaches its optimum when the prescribed spatial correlation aligns with the actual field characteristics, as evidenced by the minimum prediction error of 1.02 MPa achieved when using the correct correlation range of 100m; (3) By directly utilizing experimental variogram scatter points rather than requiring theoretical variogram model selection, the method offers remarkable flexibility while avoiding the subjective decisions typically associated with traditional variogram modeling approaches.

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