Deep Neural Networks for Large-scale Complex Spatial and Spatio-temporal Processes

PhD defense presentation by Pratik Nag
Supervised by Dr. Ying Sun (Chair)

Committee Members: Dr. Paula Moraga, Dr. Mohamed H. Elhoseiny, Dr. Veronica Berrocal

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جامعة الملك عبدالله
للعلوم والتقنية
King Abdullah University of Science and Technology

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- Project 4: Spatial Normalizing Flows for Nonstationary Gaussian Processes

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    - it involves modeling the mean and the covariance function of a spatial and spatio-temporal process.

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- Deep learning provides a computationally scalable methodology for a variety of data types and non-linear prediction. However, prediction uncertainty is an issue.

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- Project 4 proposes a generalized spatial warping function called Spatial Normalizing Flows to model complex nonstationary fields.

Project 1: Bivariate DeepKriging for Large-scale Spatial Interpolation of Wind Fields

Background

- The DeepKriging as proposed by Chen et al. (2024)[a] uses basis functions as embedding layer for the deep neural network to model the univariate spatial process.

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- This project is an extension of DeepKriging for bivariate spatial processes.

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- This project is an extension of DeepKriging for bivariate spatial processes.
- A novel data-driven prediction interval mechanism is also devised which addresses the shortcomings of the prediction interval proposed by Chen et al. (2024).

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Theory of Bivariate DeepKriging

- let $\{\mathbf{Y}(\mathbf{s}), \mathbf{s} \in D\}, D \subseteq \mathbb{R}^p$, be a bivariate spatial process. A realization of the process $\mathbf{Z}(\mathbf{s}_i)$ is modeled as $\mathbf{Z}(\mathbf{s}_i) = \mathbf{Y}(\mathbf{s}_i) + \epsilon(\mathbf{s}_i)$ with nugget $\epsilon(\mathbf{s}_i)$, observed at locations $\mathbf{s}_1, \mathbf{s}_2, \ldots, \mathbf{s}_N$.

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- The spatial model with covariates $\mathbf{X}(\mathbf{s}_i)$ can be written as $\mathbf{Y}(\mathbf{s}_i) = f(\mathbf{X}(\mathbf{s}_i)) + \gamma(\mathbf{s}_i)$, where $f(\cdot)$ is a nonlienar function and $\gamma(\mathbf{s}_i)$ is the underlying zero-mean spatial process.

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- With the above formulation the theoretical backing of Bivariate DeepKriging (**Biv.DeepKriging**) is as follows:

Theorem

For a co-located bivariate spatial process, assuming that the latent variables are constructed with the same sets of basis functions, the Linear Model of Co-regionalization (LMC)[a] represents a special case of **Biv.DeepKriging**.

[a] Genton, M. G. and W. Kleiber (2015). Cross-covariance functions for multivariate geo-statistics. Statistical Science 30 (2), 147–163.

Bivariate DeepKriging: A Spatially Dependent Deep Neural Network

- Using the multivariate Karhunen-Loéve theorem[a] the spatial process $\gamma(\mathbf{s}_i)$ can be written of the form $\gamma(\mathbf{s}_i) \approx \sum_{b=1}^{K} \{w_{b,1}\phi_{b,1}(\mathbf{s}), w_{b,2}\phi_{b,2}(\mathbf{s})\}^T$ where $w_{b,u}$'s are independent random variables and $\phi_{b,u}(\mathbf{s}_i)$'s are the pairwise orthonormal basis functions corresponding to variable u, $u = 1, 2$.

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- The idea of **Biv.DeepKriging**[c]: Through the basis function representation transform the spatial problem into a multi output regression problem by transforming the coordinate $\mathbf{s}$ to K basis functions.

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- In this work the multi-resolution compactly supported Wendland radial basis function[b] is chosen to embedd the spatial locations.
- The idea of **Biv.DeepKriging**[c]: Through the basis function representation transform the spatial problem into a multi output regression problem by transforming the coordinate $\mathbf{s}$ to K basis functions.
- We pass the covariates and the bases together $\mathbf{X}_{\phi}(\mathbf{s}_i) = (\phi(\mathbf{s}_i)^T, \mathbf{X}_{vec}(\mathbf{s}_i)^T)^T$ as input to the DNN.

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Loss Function

- The optimal neural network based predictor is obtained as $\mathbf{f}_{NN}^{opt}(\mathbf{X}_{\phi}(\mathbf{s}_0)) = \text{argmin}_{\mathbf{f}_{NN}} R(\mathbf{f}_{NN}(\mathbf{X}_{\phi}(\mathbf{s}_0))|\mathbf{Z}_{vec})$.

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- Here $R(\cdot)$ is given as

$$R\{\mathbf{f}_{NN}(\mathbf{X}_\phi(\mathbf{s}))|\mathbf{Z}_{vec}\} = \frac{1}{N}\sum_{n=1}^{N} M(\mathbf{s}_n),$$

where $M(\mathbf{s}_n) = \frac{w_1 \times (f_{NN_1}(\mathbf{X}_\phi(\mathbf{s})|\boldsymbol{\theta}) - Z_1(\mathbf{s}_n))^2 + w_2 \times (f_{NN_2}(\mathbf{X}_\phi(\mathbf{s})|\boldsymbol{\theta}) - Z_2(\mathbf{s}_n))^2}{2}$. and $w_u \propto \sigma_u^2, u = 1, 2$. We have chosen $w_u = \frac{1}{\sigma_u^2}$. Here σ_u^2 is unknown and can be estimated through the sample variance of the u-th variable.

Prediction Uncertainty (Prediction Mean)

- For the bivariate spatial prediction problem, the prediction at an unobserved location $\mathbf{s}_0$ can be expressed as

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- By employing ensembles, we can generate B replications of $\hat{\mathbf{Z}}(\mathbf{s}_0)$ at $\mathbf{s}_0$. Consequently, the prediction can be articulated as

$$\begin{aligned}\hat{\mathbf{Z}}(\mathbf{s}_0)^B &= \left(\frac{1}{B}\sum_{i=1}^{B}\hat{Z}_1(\mathbf{s}_0)_i, \frac{1}{B}\sum_{i=1}^{B}\hat{Z}_2(\mathbf{s}_0)_i\right)^T \\ &= \left(\frac{1}{B}\sum_{i=1}^{B}\left(f_{NN_1}^{opt}(\mathbf{X}_\phi(\mathbf{s}_0)) + \epsilon_1(\mathbf{s}_0)\right)_i, \frac{1}{B}\sum_{i=1}^{B}\left(f_{NN_2}^{opt}(\mathbf{X}_\phi(\mathbf{s}_0)) + \epsilon_2(\mathbf{s}_0)\right)_i\right)^T.\end{aligned}$$

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- Employing the multidimensional Central Limit Theorem $\hat{\mathbf{Z}}(\mathbf{s}_0)^B$ follows bivariate normal distribution.

Prediction Uncertainty (Prediction Variance)

- The variance term associated with $Z_u(\mathbf{s}_0)$, for $u = 1, 2$, is $\sigma^2(Z_u(\mathbf{s}_0)) = \text{Var}(Y_u(\mathbf{s}_0)) + \text{Var}(\epsilon_u(\mathbf{s}_0))$, assuming independence between $Y_u(\mathbf{s}_0)$ and $\epsilon_u(\mathbf{s}_0)$.

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- We can estimate $\text{Var}(Y_u(\mathbf{s}_0))$ as

$$\widehat{Var(Y_u(\mathbf{s}_0))} = \frac{1}{B-1}\sum_{i=1}^{B} f_{NN_u}^{opt}(\mathbf{X}\phi(\mathbf{s}_0))_i^2 - \left(\frac{1}{B}\sum_{i=1}^{B} f_{NN_u}^{opt}(\mathbf{X}_\phi(\mathbf{s}_0))_i\right)^2.$$

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- It can be shown that the noise variance will be the following

$$r_u^2(\mathbf{s}_0) = \max\{(Z_u(\mathbf{s}_0) - \frac{1}{B}\sum_{i=1}^{B} f_{NN_u}^{\text{opt}}(\mathbf{X}_\phi(\mathbf{s}_0))_i)^2 - \text{Var}\widehat{(Y_u(\mathbf{s}_0))}, 0\}.$$

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$$\widehat{Var(Y_u(\mathbf{s}_0))} = \frac{1}{B-1}\sum_{i=1}^{B} f^{opt}_{NN_u}(\mathbf{X}\phi(\mathbf{s}_0))_i^2 - \left(\frac{1}{B}\sum_{i=1}^{B} f^{opt}_{NN_u}(\mathbf{X}_\phi(\mathbf{s}_0))_i\right)^2.$$

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- Computation of $r_u^2(\mathbf{s}_0)$ as defined previously is infeasible as we do not have $Z_u(\mathbf{s}_0)$. Hence we estimate $r_u^2(\mathbf{s}_0)$ through $\hat{r}_u^2(\mathbf{s}_0) = \frac{1}{G}\sum_{\mathbf{s}_g \in D_{20}} r_u^2(\mathbf{s}_g)$, such that $\mathbf{s}_g$'s are the nearest G locations to $\mathbf{s}_0$.

Prediction Uncertainty: Prediction Interval

- Then for a given test data location $\mathbf{s}_0$ the prediction interval is

$$\hat{Z}_u(\mathbf{s}_0)^B \pm t_{(1-\alpha/2),\mathrm{df}} \sqrt{\frac{1}{B}\left(\widehat{\mathrm{Var}(Y_u(\mathbf{s}_0))} + \hat{r}_u^2(\mathbf{s}_0)\right)}, \; u = 1, 2,$$

where $t_{(1-\alpha/2),\mathrm{df}}$ represents the $1-\alpha/2$ quantile of the t-distribution with df degrees of freedom, $\mathrm{df} = N - p$, where p denotes the number of estimated parameters.

Algorithm for Prediction Interval

Algorithm 1 Prediction Intervals Algorithm

Split $\mathbf{D}$ into $\mathbf{D_1}$ and $\mathbf{D_2}$ equally.
Further split $\mathbf{D_1}$ into $\mathbf{D_{11}}$ and $\mathbf{D_{12}}$.
Train a deep neural network (**DNN**) of L layers on $\mathbf{D_{11}}$.
Take $\mathbf{B}$ random samples $\{\mathbf{D_1^1}, \mathbf{D_1^2}, ..., \mathbf{D_1^B}\}$ from $\mathbf{D_1}$.
for $i \leftarrow 1$ to $\mathbf{B}$ **do**
    Fix the weights of the first L_0 layers of the **DNN** and train the last $L - L_0$ layers on $\mathbf{D_1^i}$.
    Train the **DNN** on $\mathbf{D_1^i}$ and store the result. Denote it as $\mathbf{f}_{NN}^{opt}(\mathbf{X}_\phi(\mathbf{s}))_i$.
end for
for location $\mathbf{s}_k$ in $\mathbf{D_2}$ **do**
    Calculate $\hat{Z}_u(\mathbf{s}_k)^B$(6) and $\widehat{Var(Y_u(\mathbf{s}_k))}$ (7).
    Calculate $r_u^2(\mathbf{s}_k)$ (8).
end for
For test location $\mathbf{s}_0$, obtain the set $\mathbf{D_{20}} = \{\mathbf{s}_k : \mathbf{s}_k \in \mathbf{D_2}\}$ of the nearest G locations from $\mathbf{s}_0$.
Calculate $\hat{Z}_u(\mathbf{s}_0)^B$(6), $\widehat{Var(Y_u(\mathbf{s}_k))}$ (7), and $\hat{r}_u^2(\mathbf{s}_0)$ (10).
Calculate the prediction interval as defined in (9).
$\triangleright$ Where u stands for the u-th variable, $u = 1, 2$.

Simulation Studies

- Three separate simulation scenarios are devised:
    - Gaussian with parsimonious Matérn covariance.
    - Non-Gaussian process with covariates : Gaussian process is generated and it is then transformed by the Tukey G and H transformation to yield non-Gaussian field
    - Nonstationary process : Nonlinear combinations of basis functions are taken into consideration for this process generation.
- Each simulation scenario is replicated 100 times.

Simulation Studies

The proposed model (**Biv.DeepKriging**) is compared against Gaussian kriging with parsimonious Matérn covariance(**CoKriging.Matérn**) and Linear Model of Coregionalization (**CoKriging.LMC**) respectively.

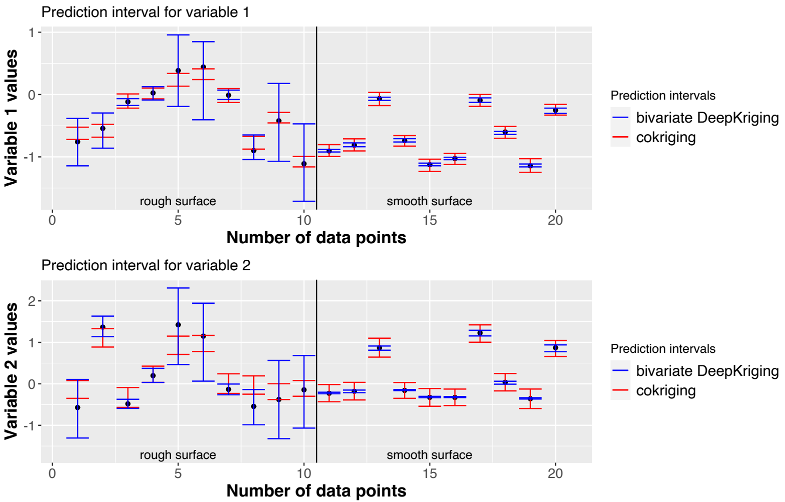
Different metrics such as the Mean Square Prediction Error (MSPE), Prediction Interval Coverage Probability (PICP) and Mean Prediction Interval Width (MPIW) are considered for comparing the predictions and the prediction intervals.

Table: Comparison on both the variables over different simulation settings.

Simulation type	Models	**MSPE$_1$**	**SE$_1$**	**PICP$_1$**	**MPIW$_1$**	**MSPE$_2$**	**SE$_2$**	**PICP$_2$**	**MPIW$_2$**
Gaussian	**CoKriging.Matérn$_{true}$**	0.23	0.11	0.95	0.87	0.21	0.09	0.95	0.92
	Biv.DeepKriging	0.24	0.19	0.94	0.98	0.24	0.18	0.95	1.07
non-Gaussian	**CoKriging.Matérn**	3.48 ($\times10^3$)	0.29 ($\times10^3$)	0.27	6.21	0.98 ($\times10^3$)	0.49 ($\times10^3$)	0.26	6.16
	CoKriging.LMC	87.4	12.13	0.58	11.2	94.5	21.9	0.51	9.99
	Biv.DeepKriging	32.7	11.6	0.94	29.9	23.8	9.11	0.94	29.4
non-stationary	**CoKriging.Matérn**	1.95	0.75	0.92	3.53	0.13	0.02	0.09	1.01
	CoKriging.LMC	1.26	0.14	0.92	3.49	0.14	0.02	0.10	1.33
	Biv.DeepKriging	7.52 ($\times10^{-4}$)	1.01 ($\times10^{-4}$)	0.96	0.16	6.83 ($\times10^{-4}$)	1.08 ($\times10^{-4}$)	0.95	0.19

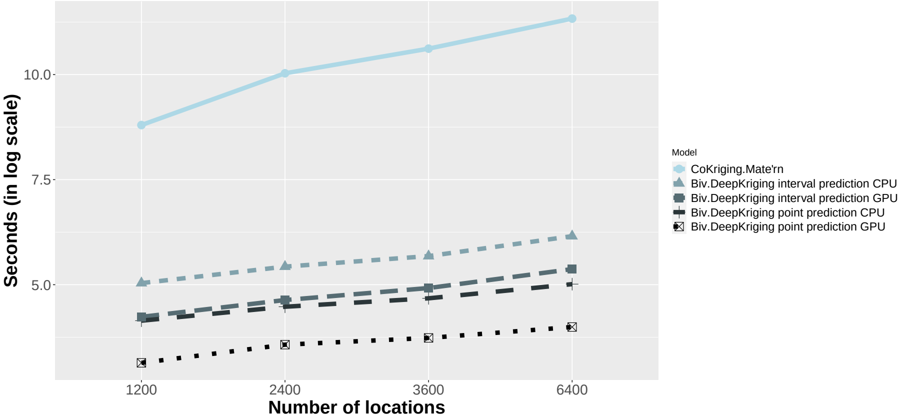
Simulation studies: Prediction intervals

Figure: Prediction interval for variable 1 and variable 2 for the nonstationary simulation.



Simulation Studies: Computation Time

Figure: Total computation time (in secconds) for different models in log scale for different number of locations



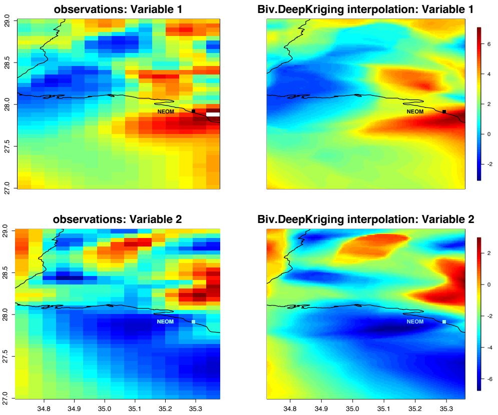
Application on Wind Data

- The U and V components of wind over the Middle East, encompassing 506,771 locations, are considered for this study.
- For **CoKriging.Matérn** total computation time was 2.18 days where as for **Biv.DeepKriging** it took **16.81 minutes** for point prediction and **55.61 minutes** for interval prediction.

Models	$\mathbf{RMSPE}_1$	$\mathbf{RMSPE}_2$
CoKriging.Matérn	0.882	4.066
Biv.DeepKriging$_{147000}$	0.488	0.438
Biv.DeepKriging$_{450000}$	**0.394**	**0.392**

Models	$PICP_1$	$PICP_2$	$MPIW_1$	$MPIW_2$
CoKriging.Matérn	0.601	0.734	1.671	1.343
Biv.DeepKriging	**0.971**	**0.950**	**1.226**	**1.340**

Spatial Downscaling



- A high resolution interpolation is given ($1km \times 1km$) for the region near NEOM, an upcoming smart city in Saudi Arabia. This downscaling can help understand the wind pattern better and can potentially help in wind energy setup in the area.

Conclusion

- The proposed framework, **Biv.DeepKriging**, which generalizes the Linear Model of Coregionalization, is suitable for modeling bivariate non-Gaussian and nonstationary spatial fields.

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Conclusion

- The proposed framework, **Biv.DeepKriging**, which generalizes the Linear Model of Coregionalization, is suitable for modeling bivariate non-Gaussian and nonstationary spatial fields.
- The proposed method is also computationally scalable and can be implemented for large-scale datasets.
- The proposed prediction interval technique does not rely on the distribution of the data and can be applied to any kind of application beyond spatial modeling.

Project 2: Spatio-Temporal DeepKriging for Probabilistic Interpolation and Forecasting

Background

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- Consider the real valued spatio-temporal random field $\{Y(\mathbf{s}, t), \mathbf{s} \in D, t \in \mathcal{T}\}, D \subseteq \mathbb{R}^p, \mathcal{T} \subseteq \mathbb{R}$. Assuming the data is observed at N locations and K time points, the realizations can be given as $\mathbf{Z}_{N,K} = \{Z(\mathbf{s}_1, t_1), Z(\mathbf{s}_2, t_1), \dots, Z(\mathbf{s}_N, t_K)\}$ such that

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$$Z(\mathbf{s}_i, t_j) = Y(\mathbf{s}_i, t_j) + \epsilon(\mathbf{s}_i, t_j).$$

- Given observations $\mathbf{Z}_{N,K}$, two common goals of spatio-temporal prediction are probabilistic interpolation, i.e., predict the true process $Y(\mathbf{s}_0, t)$ at unobserved spatial location $\mathbf{s}_0$, and forecasting, i.e., predict $Y(\mathbf{s}_0, t_{K+u})$ at unobserved location $\mathbf{s}_0$ at a future time point t_{K+u}.

Optimal Predictor for Probabilistic Interpolation

- The optimal predictor can written as:

$$\hat{Y}_{\tau}^{opt}((\mathbf{s}_0, t)|\mathbf{Z}_{N,K}) = \underset{\hat{Y}}{\text{argmin}}\, R_1(\hat{Y}_{\tau}(\mathbf{s}_0, t)|\mathbf{Z}_{N,K}),$$

where $R_1(\cdot)$ represents the true risk function necessary for obtaining the τ-th quantile prediction.

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- An estimation for $R_1(\cdot)$ can be expressed through the quantile loss function, defined as:

$$R_1^{emp}(\hat{Y}_\tau(\mathbf{s}, t)|\mathbf{Z}_{N,K}) = \frac{1}{NK}\sum_{n=1}^{N}\sum_{k=1}^{K}\rho_\tau(\hat{Y}_\tau(\mathbf{s}_n, t_k) - Z(\mathbf{s}_n, t_k)),$$

where $\rho_\tau(v) = v(\tau - I(v < 0))$ and $\tau \in (0, 1)$ is quantile level.

Space-Time.DeepKriging: DNN for Interpolation

- Similar to DeepKriging[a] a single-output deep neural network structure (**Space-Time. DeepKriging**) is used to build the spatio-temporal DeepKriging framework with basis functions as inputs.

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- Wendland's compactly supported radial basis functions are used for spatial location embedding and Gaussian radial bases are used for temporal embedding.
- Hence $\hat{Y}_\tau(\cdot,\cdot)$ can be expressed through the DNN as:

$$\hat{Y}_\tau(\mathbf{s}, t) = \Psi(\tau, f_{NN_\tau}(\mathbf{X}_\phi(\mathbf{s}, t))),$$

where $\mathbf{X}_\phi(\mathbf{s}, t)$ is the set of stacked basis functions, $f_{NN_\tau}(\mathbf{X}_\phi(\mathbf{s}, t))$ is the DNN output at quantile level τ, and $\Psi(\cdot,\cdot)$ is the activation function of the output layer.

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The Output Layer Activation $\Psi(\cdot,\cdot)$

- In theory, quantile regression lines are expected not to intersect; however, unconstrained optimization of $R_1^{emp}(\hat{Y}_\tau(\mathbf{s},t)|\mathbf{Z}_{N,K})$ may inadvertently introduce crossing issues.

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- To avoid quantile cross-over, the following activation function for the output layer is proposed:

$$\Psi(\tau, x) = \begin{cases} x & \text{for } \tau = 0.5 \\ f_{Constant} + \frac{\lambda(\tau - 0.5)}{1+e^{-x}} & \text{for } \tau > 0.5 \\ f_{Constant} - \frac{\lambda(0.5-\tau)}{1+e^{-x}} & \text{for } \tau < 0.5, \end{cases}$$

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- Here $f_{Constant}$ is the model output for quantile level 0.5, λ is the hyperparameter proportional to the variance of the data.

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- Although **QLSTM** is highly effective for capturing temporal dependence, it does not use information from other locations.
- For space-time data, this project propose the convolutional LSTM which includes data from other locations by passing the CNN layer as the input to the LSTM layer (call it **QConvLSTM**).

Optimal Predictor for **QConvLSTM**

- The optimal predictor can written as:

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- Note that, the input to $f_{NN_{\tau}}^{Conv}(\mathbf{s}_0, t_k)$ here is:
  $\mathbf{X}^{NN_{CONV}} = \{\mathcal{A}(\mathbf{s}_0, t_1), \ldots, \mathcal{A}(\mathbf{s}_0, t_K)\}$, where $\mathcal{A}(\mathbf{s}_0, t_k)$ is a $r \times r$ matrix of interpolation over a gridded neighbourhood $N_{\mathbf{s}_0}$ around $\mathbf{s}_0$.

Simulation Studies

- The proposed **Space-Time.DeepKriging** won the KAUST competition in large-scale prediction on 100k and 1M space-time locations with double digit improvement in percentage for MSPE over competing methods such as the Veccia's approximation and block composite likelihood.

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- We compare the method on a simulated nonstationary field with 50k space-time locations with other competitive methods that can be applied for large-scale interpolation and forecasting.

Numeric Results on Simulated Data

Table: Average MSPE of prediction for simulated data. Here SE stands for standard error of the predictions.

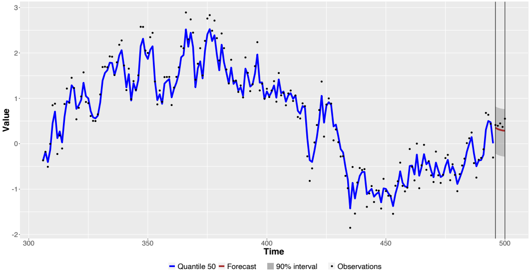
Models	MSPE	SE
Space-Time.DeepKriging	0.167	0.073
GpGp	0.746	0.288

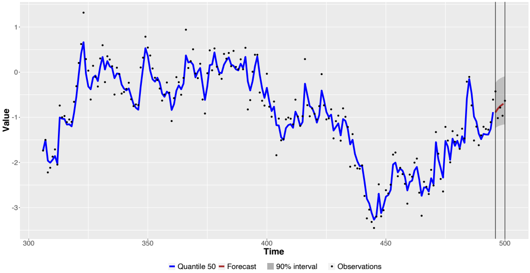
Table: Average MSPE, MPIW and PICP of forecast for simulated data.

Models	Avg.MSPE	SE	Avg.MPIW	SE	Avg.PICP
QConvLSTM	0.267	0.219	1.462	0.126	90.39
ARIMA	0.277	0.278	2.262	0.082	90.72
QLSTM	0.392	0.523	1.558	0.316	89.94
GpGp	0.839	0.358	-	-	-

Forecast on Simulated Data

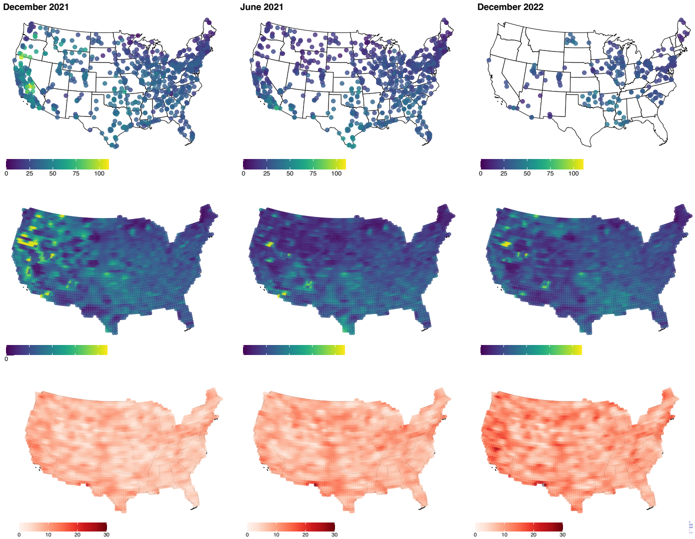
- Forecasting at specific observed locations using **QConvLSTM**.





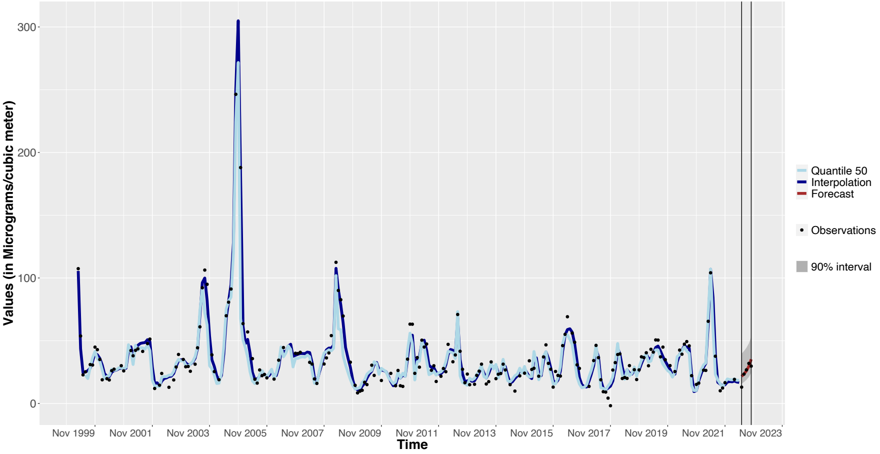
Application on $PM_{2.5}$: Interpolation

We also apply our method to the $PM_{2.5}$ data over USA with over 200,000 space-time locations.



Application on $PM_{2.5}$: Forecast for San Francisco

Forecast period for the last six observed months up to December 2022:



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- The proposed method for spatio-temporal interpolation and forecasting is valid for general class of non-Gaussian and nonstationary spatio-temporal processes.

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- The proposed method for spatio-temporal interpolation and forecasting is valid for general class of non-Gaussian and nonstationary spatio-temporal processes.
- The proposed approach can be easily extended to large datasets with minimum hardware support.

Project 3: Efficient Large-scale Nonstationary Spatial Covariance Function Estimation using Convolutional Neural Networks

Introduction

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- In environmental and ecological applications nonstationarity assumption is more realistic and can be accounted through Covariance Nonstationarity.
- This project gives a novel approach for modeling the nonstationary Matérn covariance function through HPC and convolutional neural networks.

Nonstationary Matérn Covariance Function

- Let $Z(\cdot)$ be a spatial process observed over locations $\mathbf{s}_1, \mathbf{s}_2, \ldots, \mathbf{s}_N \in D \subseteq \mathbb{R}^d$, where $Z(\mathbf{s}_i) = \mu(\mathbf{s}_i) + Y(\mathbf{s}_i) + \epsilon, \mathbf{s}_i \in D$ with the underlying GRF $Y(\mathbf{s}_i)$ having covariance function $C(\cdot, \cdot)$.

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- The nonstationary Matérn covariance:

$$C^{NS}(\mathbf{s}_i, \mathbf{s}_j; \boldsymbol{\theta}) = \tau(\mathbf{s}_i)\tau(\mathbf{s}_j)\mathbb{1}_{ij}(\mathbf{s}_i, \mathbf{s}_j) + \frac{\sigma(\mathbf{s}_i)\sigma(\mathbf{s}_j)|\Sigma(\mathbf{s}_i)|^{1/4}|\Sigma(\mathbf{s}_j)|^{1/4}}{\Gamma(\bar{\nu}(\mathbf{s}_i, \mathbf{s}_j))2^{\bar{\nu}(\mathbf{s}_i, \mathbf{s}_j)-1}}$$
$$\times \left|\frac{\Sigma(\mathbf{s}_i) + \Sigma(\mathbf{s}_j)}{2}\right|^{-1/2} \left(2\sqrt{\bar{\nu}(\mathbf{s}_i, \mathbf{s}_j)Q_{ij}}\right)^{\bar{\nu}(\mathbf{s}_i, \mathbf{s}_j)} \mathcal{K}_{\bar{\nu}(\mathbf{s}_i, \mathbf{s}_j)}\left(2\sqrt{\bar{\nu}(\mathbf{s}_i, \mathbf{s}_j)Q_{ij}}\right),$$

and $\nu_{ij} = \frac{\nu(\mathbf{s}_i)+\nu(\mathbf{s}_j)}{2}$, where $\boldsymbol{\theta}(\mathbf{s}_i) = \{\Sigma(\mathbf{s}_i), \sigma(\mathbf{s}_i), \tau^2(\mathbf{s}_i), \nu(\mathbf{s}_i)\}$ are spatially varying parameters that control nonstationarity.

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- $\Sigma(\mathbf{s}_i)$ controls the spatial range and anisotropy, $\sigma(\mathbf{s}_i)$ controls the local standard deviation, $\tau^2(\mathbf{s}_i)$ controls the nugget effect, and $\nu(\mathbf{s}_i)$ controls the smoothness.

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- $Q_{ij} = (\mathbf{s}_i - \mathbf{s}_j)^T \left(\frac{\Sigma_i+\Sigma_j}{2}\right)^{-1} (\mathbf{s}_i - \mathbf{s}_j)$ is the Mahalanobis distance between points $\mathbf{s}_i$ and $\mathbf{s}_j$.

Existing Methods and Challenges

- Existing methods:

[a] Risser MD, Calder CA (2017). "Local Likelihood Estimation for Covariance Functions with Spatially-Varying Parameters: The convoSPAT Package for R." Journal of Statistical Software, 81(14), 1–32. doi:10.18637/jss.v081.i14.

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Maximum Likelihood Parameter Estimation with ExaGeoStat

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- `ExaGeoStat` estimates the statistical parameters of a given geospatial domain in parallel and at large-scale. `ExaGeoStat` has distributed memory support, enabling one to perform parallel computing.

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- Let K represent the total number of subregions and $\mathbf{S}_1, \mathbf{S}_2, ..., \mathbf{S}_K$ be the anchor locations to those subregions, which are the centers of different subregions. The spatially varying parameters are defined as:

$$\boldsymbol{\theta}(\boldsymbol{s}_i) = \sum_{k=1}^{K} W(\boldsymbol{s}_i, \boldsymbol{S}_k)\, \boldsymbol{\theta}(\boldsymbol{S}_k).$$

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- For any $\mathbf{s}_i \in D \subset \mathbb{R}^d$, where $\mathbf{S}_k$'s are anchor locations and $\boldsymbol{\theta}(S_k)$'s are the parameter values at those anchor locations.

$$W\left(\mathbf{s}_i, \boldsymbol{S}_k\right) = \frac{K\left(\mathbf{s}_i, \boldsymbol{S}_k\right)}{\sum_k K\left(\mathbf{s}_i, \boldsymbol{S}_k\right)}$$

and the Gaussian kernel $K\left(\mathbf{s}_i, \boldsymbol{S}_k\right) = exp\left(\left(-\|\mathbf{s}_i - \boldsymbol{S}_k\|^2\right)/2h\right)$, where h is the bandwidth.

ConvNet for Nonstationarity Classification

- This project propose a Convolutional Neural Network based classifier (**ConvNet**) which can be used to distinguish between stationary and nonstationary random fields.

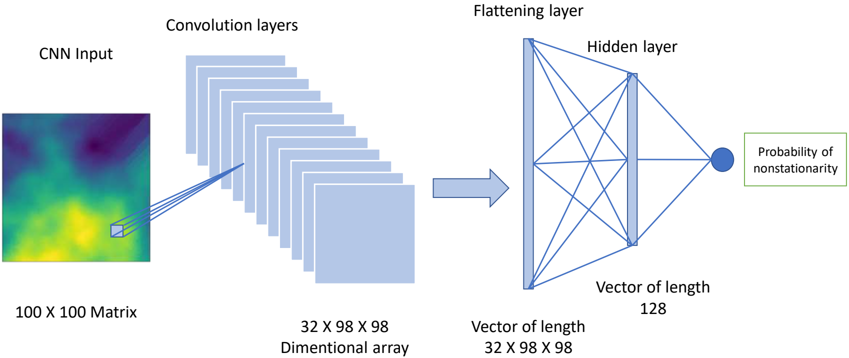

Figure: The structure of the CNN model, the flatten layer victories the CNN layer output, the final layer with softmax activation provides the probability of a particular class.

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- A simple pre-processing transformation is followed to transform the data into a regular 100×100 grid.

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- This process is followed for B number of iterations.
- The optimal cluster is then chosen for which the combined nonstationarity index as obtained from the **ConvNet** model is the smallest.

Simulation Studies : Performance of The **ConvNet** Model

The **ConvNet** model obtains 97% and 98% accuracy respectively in successfully identifying the stationary and nonstationary random fields on test data.

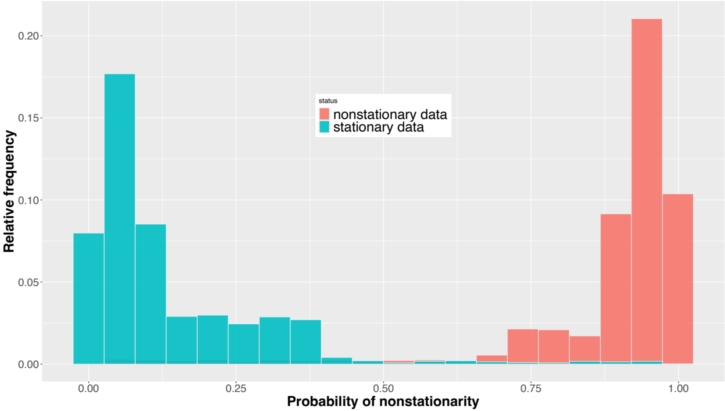

Figure: Histogram of the nonstationarity index for stationary testing data and nonstationary testing data.

Simulation Study: Parameter Estimation

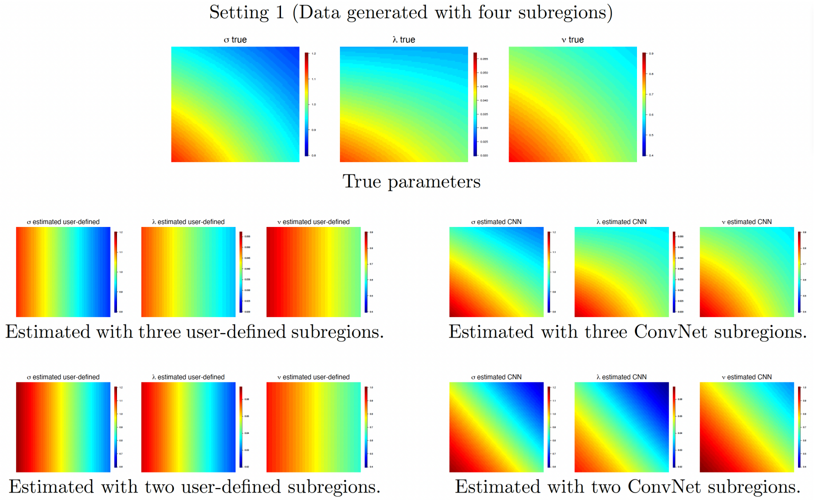

Figure: Heatmaps for true parameters and the average of the estimated parameters for different simulation scenarios.

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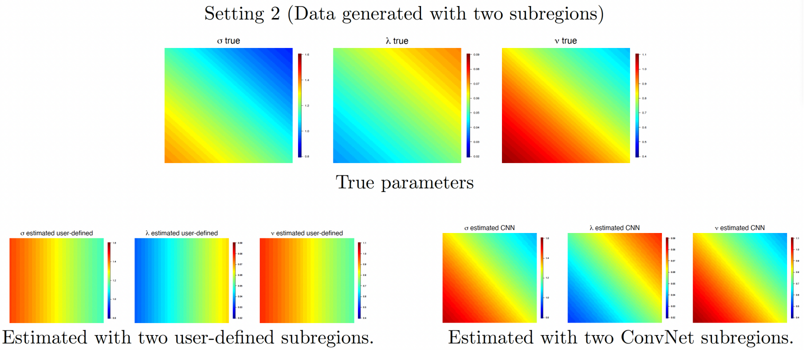

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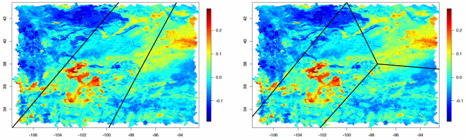
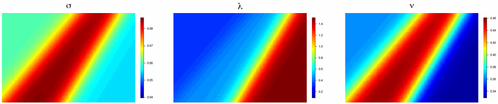
Soil Moisture Data Application

This method is applied to analyze soil moisture content data across the Mississippi Basin region in the United States with 200,000 locations. Based on AIC the performing model came out to be the three-subregion model.

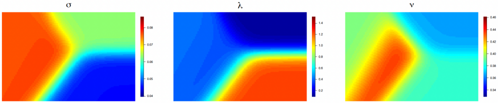
Soil Moisture Data



The black lines show the splits for three and four subregions, respectively.



Estimated with three ConvNet subregions.



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- This project present **ConvNet**, an approach that is able to distinguish the stationary and nonstationary regions.

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- **ConvNet** is then coupled with a clustering mechanism to identify the stationary subregions in a given geospatial region.
- `ExaGeoStat` framework is used along with the clustering mechanism for exact large-scale implementation of nonstationary Matérn kernel.

Project 4: Spatial Normalizing Flows for Nonstationary Gaussian Processes

Background

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- Modeling complex environmental phenomena often involves selecting nonstationary and anisotropic covariance structures such as the non-stationary Matérn covariance as discussed in previous section.
- However, the choise of the covarince can pose challenges when the underlying spatial process is not well-understood.
- An alternative approach to model these intricate structures involves deformation of the spatial domain with the idea that a process that is highly nonstationary or anisotropic on the original domain could be stationary and isotropic on the warped domain.

Existing Methods and Challenges

- Key previous works:

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- This work explores the novel application of Neural Autoregressive Flows (NAFs) to model spatial warping.

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The normalizing flow (NF) is an invertible function typically used to model transformations of random variables. We employ the normalizing flow to warp the spatial locations. A special type of NF is the auto-regressive flow (AF) which can be viewed as a triangular map $\boldsymbol{T}(.)$ where

$$T^{(k)}(s_1, \ldots, s_k) = S^{(k)}(s_k; \gamma_k(s_1, \ldots, s_{k-1}; \boldsymbol{\vartheta}_k)),$$

where, $\{s_1, \ldots, s_k\} \subseteq \mathbf{s}, k = 1, \ldots, d$, and γ_k is the k-th conditional network with parameters $\boldsymbol{\vartheta}_k$. The conditional network is a multivariate mapping that takes inputs $s_1, \ldots, s_{k-1}$ and gives outputs in the parameter space of $S^{(k)}$, i,e., $\gamma_k : D^{k-1} \rightarrow \mathbb{R}^{m_k}$, where m_k is the number of parameters that parameterize $S^{(k)}$.

Normalizing Flows

This work focuses on the class of Neural Autoregressive Flows (NAFs), proposed by Huang et al. (2018)[a]. We choose a class of functions commonly referred to as Deep Sigmoidal Flows (DSF). In this class, one single layer has $m_k = 3M$ parameters, where $M \geq 1$, and the k-th component has the form

$$S^{(k)}(s_k; \gamma_k) = \sigma^{-1}\left(\boldsymbol{w}_k^T \sigma(\boldsymbol{a}_k s_k + \boldsymbol{b}_k)\right),$$

where $\sigma^{-1}(\cdot)$ is the logit function and parameters $\gamma_k \equiv (\boldsymbol{w}_k^T, \boldsymbol{a}_k^T, \boldsymbol{b}_k^T)^T$ are neural network functions of length M with $\sum_{i=1}^{M} w_{ki} = 1$. This construction ensures monotonicity of the function $S^{(k)}(\cdot)$ and hence of the function $T^{(k)}(\cdot)$. Ultimately, this construction ensures that the multivariate mapping $\boldsymbol{T}(s_1, \ldots, s_k)$ will be injective.

[a] Huang, C.-W., D. Krueger, A. Lacoste, and A. Courville (2018). Neural autoregressive flows. In International Conference on Machine Learning, pp. 2078–2087. PMLR.

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- The alternative framework is the Deep Dense Sigmoidal Flows (DDSFs). In this class, layer l of the flow has $m_k = M_l^2 + M_l M_{l-1} + 2M_l$ parameters, where $M_{l-1}, M_l \geq 1$ with

$$\begin{aligned} h_k^1 &= \sigma^{-1}\left(\boldsymbol{w}_k^1 \sigma(\boldsymbol{a}_k^1 \odot (\boldsymbol{u}_k^1 s_k) + \boldsymbol{b}_k^1)\right), \\ h_k^{l-1} &= \sigma^{-1}\left(\boldsymbol{W}_k^l \sigma(\boldsymbol{a}_k^l \odot (\boldsymbol{U}_k^l \boldsymbol{h}_k^{l-1}) + \boldsymbol{b}_k^l)\right), \quad l = 2, \ldots, L-1, \\ h_k^L &= \sigma^{-1}\left(\boldsymbol{w}_k^L \sigma(\boldsymbol{a}_k^L \odot (\boldsymbol{u}_k^L h_k^{L-1}) + \boldsymbol{b}_k^1)\right), \end{aligned}$$

$$S^{(k)}(s_k; \gamma_k) = h_k^L,$$

where, $\sum_{j=1}^{M_l} w_{kij} = 1$ and $\sum_{j=1}^{M_l} u_{kij} = 1$ corresponding to the i-th row of matrices $\boldsymbol{W}_k^l, \boldsymbol{U}_k^l$. Similar to DSF the parameters here are defined through γ_k.

Binary Masking

- The vector of locations $\mathbf{s}$ is passed through a single feed forward network to obtain γ_k. To enforce the autoregressive property, the feed forward function is modified by introducing binary mask $\mathbf{M_W}$:

$$\gamma_k = \boldsymbol{g}\left(\mathbf{b} + \left(\mathbf{W} \odot \mathbf{M_W}\right)\mathbf{s}\right)$$

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- Constraints on the maximum number of inputs to each hidden unit are encoded in the matrix masking the connections between input and hidden units:

$$M_{\mathbf{W}_{j,k}} = 1_{m(j) \geq k} = \begin{cases} 1 & \text{if } m(j) \geq k \\ 0 & \text{otherwise} \end{cases},$$

  for $k \in \{1, \ldots, D\}$ and $l \in \{1, \ldots, L\}$. Overall, the constraint is that the k^{th} output unit connects only to $\mathbf{s}_{<k}$ (not to $\mathbf{s}_{\geq k}$).

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- $$Y^{(1,2)}(s) = \begin{cases} \exp\left(4 + \frac{5}{2s(10s+5)}\right) & -0.5 < s < 0 \\ 1 & 0.2 \leq s \leq 0.3 \\ -1 & 0.3 < s \leq 0.4 \\ 0 & \text{otherwise.} \end{cases}$$

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- Two dimentional :

  The warping function SWGIP as proposed in Zammit-Mangion et al. (2021)[a] is taken and compared with other approaches. Data is simulated in two dimensions from the underlying SIWGP on $G = [-0.5, 0.5]^2$, denoted as $Y^{(2,1)}(\cdot)$.

[a]Zammit-Mangion, A., Ng, T. L. J., Vu, Q. and Filippone, M. (2021) Deep compositional spatial models. Journal of the American Statistical Association pp. 1–22.

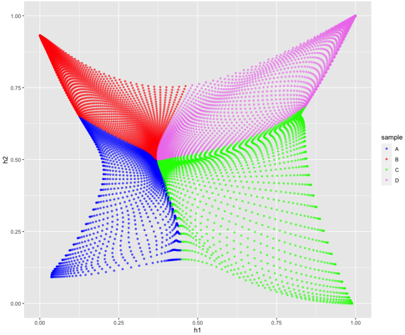
Simulation Studies: Results

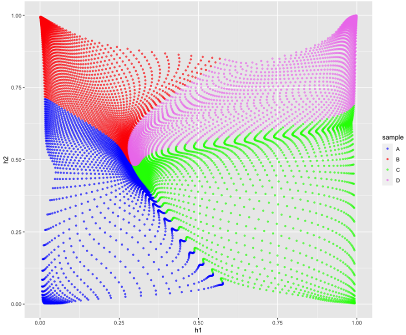
Table: Comparison on different simulation scenarios.

dataset	Models	**MSPE**	**PICP**	**MPIW**
$Y^{(1,1)}(s)$	$GP_{nonstat}$	0.033	0.93	0.47
	GP_{orig}	0.034	0.94	0.47
	GP_{warped}	0.033	0.94	0.45
$Y^{(1,2)}(s)$	$GP_{nonstat}$	0.021	0.90	0.522
	GP_{orig}	0.025	0.90	0.521
	GP_{warped}	0.016	0.93	0.423
$Y^{(2,1)}(\mathbf{s})$	$GP_{nonstat}$	0.348	0.96	2.822
	GP_{orig}	0.372	0.97	2.833
	GP_{warped}	0.063	0.97	1.171

The Estimated Warping in 2-dimension

The true (left) and the estimated (right) warpings for $Y^{(2,1)}(\cdot)$.





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Conclusion

- Spatial normalizing flow represents a deep-learning-based model that excels in handling processes featuring highly complex nonstationary and anisotropic covariance structures.
- Its construction inherently imposes a smooth injective constraint, thereby limiting the class of warpings and effectively mitigating the issue of "space-folding."
- This method boasts extendability to higher dimensions, as the Neural Autoregressive Flows (NAF) architecture seamlessly accommodates multidimensional mappings.

Publications: Thesis Works

- **Pratik Nag**, Ying Sun, Brian J Reich. *Spatio-temporal DeepKriging for Interpolation and Probabilistic Forecasting*, Spatial Statistics (Oct, 2023), volume. 57, 100773, DOI 10.1016/j.spasta.2023.100773.
- **Pratik Nag**, Ying Sun, Brian J Reich. *Bivariate DeepKriging for Computationally Efficient Spatial Interpolation of Large-scale Wind Fields*, Arxiv : https://arxiv.org/abs/2307.08038.(In Revision at Technometrics).
- **Pratik Nag**, Sameh Abdulah, Yiping Hong, Ghulam Qadir, Ying Sun, Marc G. Genton. *Efficient Large-scale Nonstationary Spatial Covariance Function Estimation Using Convolutional Neural Networks*, Arxiv : https://arxiv.org/abs/2306.11487. (In Revision at Journal of Computational and Graphical Statistics (JCGS)).
- **Pratik Nag**, Andrew Zammit-Mangion, Ying Sun. *Spatial Normalizing Flows for Nonstationary Gaussian Processes*(in preparation).

Publications: Other Works

- **Pratik Nag**, Arnab Hazra, Rishikesh Yadav, Ying Sun. *Exploring the Efficacy of Statistical and Deep Learning Methods for Large Spatial Datasets: A Case Study*, JABES (2024). https://doi.org/10.1007/s13253-024-00602-4
- Sameh Abdulah, Faten Alamri, **Pratik Nag**, Ying Sun, Hatem Ltaief, David E. Keyes, Marc G. Genton, *The Second Competition on Spatial Statistics for Large Datasets*, J. data sci.(2022), 1-22, DOI 10.6339/22-JDS1076.
- Qinglei Cao, Sameh Abdulah, Rabab Alomairy,Yu Pei, **Pratik Nag**, George Bosilca, Jack Dongarra, Marc G. Genton,David E. Keyes, Hatem Ltaief, Ying Sun. *Reshaping Geostatistical Modeling and Prediction for Extreme-Scale Environmental Applications*, In2022 SC22: International Conference for High Performance Computing, Networking, Storage and Analysis (SC) 2022 Nov 3 (pp. 13-24). IEEE Computer Society.(Finalist for **Gordon Bell Prize**).
- **Pratik Nag**, Huixia Judy Wang, Ying Sun. *Indicator DeepKriging for Probabilistic Prediction of Spatial Processes*(in preparation).

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