Deep Gaussian Processes for Air Quality Inference

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ABSTRACT
Air pollution kills around 7 million people annually, and approximately 2.4 billion people are exposed to hazardous air pollution. Accurate, fine-grained air quality (AQ) monitoring is essential to control and reduce pollution. However, AQ station deployment is sparse, and thus air quality inference for unmonitored locations is crucial. Conventional interpolation methods fail to learn the complex AQ phenomena. This work demonstrates that Deep Gaussian Process models (DGPs) are a promising model for the task of AQ inference. We implement Doubly Stochastic Variational Inference, a DGP algorithm, and show that it performs comparably to the state-of-the-art models.

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1 INTRODUCTION
Air pollution causes fine particulate matter which results in strokes, heart diseases, lung cancer, and acute and chronic respiratory diseases. Accurate fine-grained monitoring of air quality can help mitigate air pollution. The air quality monitoring stations are expensive to install and maintain. In this paper, we study AQ inference to estimate AQ at unmonitored locations.

Prior works like ADAIN [3] have leveraged attention-based mechanisms to estimate AQ. But, the deep neural network cannot capture the notion of uncertainty. This limitation can be solved by using non-parametric probabilistic machine learning techniques such as Gaussian Processes (GPs) [10]. The ability of GPs to capture domain knowledge while predicting makes them advantageous over deep learning methods. Hence, GPs play a crucial role in certain applications where intuitive risk assessments are needed [14]. However, GPs are limited by issues such as scalability [8] and the inability to extract hierarchical features [7].

Environmental phenomena exhibit non-stationarity (dynamic mean and covariance matrix) and complex inter-variable relationships. However, if we use stationary GPs, we need to parameterise the discontinuities, which becomes a problem if we do not know the number of discontinuities and do not wish to specify where they occur. In Deep Gaussian Processes (DGPs), we can obtain a non-parametric representation of discontinuities since the models are not restricted to Gaussian processes, and the covariance function can have non-Gaussian characteristics [1]. DGPs are multi-layer hierarchical generalisations of GPs, comparable to neural networks with numerous, indefinitely large hidden layers. DGPs are probabilistic and non-parametric, making them more generalizable, and capable of providing better-calibrated uncertainty estimates than other deep models.

Prior literature [4] has shown that DGPs have outperformed GPs on several known datasets, thus encouraging us to endeavour this approach for AQ inference. Further, prior work [13] shows that their proposed method, Doubly Stochastic Variational Inference (DSVI) algorithm, a DGP model, works well in practice on different classification and regression tasks. For the regression task on the UCI Elevators Dataset, we found that DGP model outperforms the Gaussian Processes [11] model and other baselines. DSVI has also been proven [13] to work well for other large-scale regression tasks, this motivated us to pursue DSVI for air quality inference on the Beijing Dataset.

Our experiments show promise in that the air quality inference can be improved by combining the ardent power of deep learning with GPs in one expressive Bayesian learning model.

2 APPROACH
We implement the Doubly Stochastic Variational Inference (DSVI) model which incorporates sparsity, stochastically approximates the Bayesian model and returns a posterior using Variational Inference. Sparse variational inference employs inducing points to simplify the complex correlation between the DGP layers. While evaluation, the model takes random samples from univariate Gaussians.

We use GPyTorch [5] to build a DSVI Deep Gaussian model. We use the Squared Exponential (RBF) kernel and the VariationalELBO loss function. The layers also have “skip connections” between them, similar to ResNet [6].

3 EVALUATION
3.1 Experimental Setup
The dataset comprises of hourly PM$_{2.5}$ (major pollutant) data from 36 air quality monitoring stations located in Beijing city along with meteorological data (temperature, weather, humidity, wind direction and pressure). The dataset is available for duration of a year from 1st May 2014 to 30th April 2015. Following previous works [3, 11] we use 3-fold cross validation. We perform hyperparameter tuning using grid search on inducing
We now discuss the future work to overcome the limitations. We identify the following areas where the model can be improved: i) Figure 1 shows that the model is able to capture low-frequency signals correctly but is unable to predict the high-frequency signals accurately. 2) Also, we are not able to detect uncertainty band near the peaks.

![Figure 1: Predicted PM$_{2.5}$ comparison with the ground truth values for DSVI model at station 1006](image_url)

**4 FUTURE WORK**

We now discuss the future work to overcome the limitations. We can improve the predictions by i) using combinations of kernels ii) designing kernels pertaining to specific features [11]. iii) using calibration to better capture the notion of uncertainty and iv) increasing the number of layers to further exploit the advantages of DGPs and tune the hyperparameters accordingly.

**REFERENCES**

[1] Leo Breiman. 2001. Random forests. Machine learning 45, 1 (2001), 5–32.
[2] Tianqi Chen and Carlos Guestrin. 2016. Xgboost: A scalable tree boosting system. In Proceedings of the 22nd acm sigkdd international conference on knowledge discovery and data mining. 785–794.
[3] Weiyu Cheng, Yanyan Shen, Yamin Zhu, and Linpeng Huang. 2018. A neural attention model for urban air quality inference: Learning the weights of monitoring stations. In Proceedings of the AAAI Conference on Artificial Intelligence, Vol. 32.
[4] Andreas Damianou and Neil D Lawrence. 2013. Deep gaussian processes. In Artificial intelligence and statistics. PMLR, 207–215.
[5] Jacob R Gardner, Geoff Pleiss, David Bindel, Kilian Q Weinberger, and Andrew Gordon Wilson. 2018. GPYtorch: Blackbox Matrix-Matrix Gaussian Process Inference with GPU Acceleration. In Advances in Neural Information Processing Systems.
[6] Kaiming He, Xiangyu Zhang, Shaoqing Ren, and Jian Sun. 2016. Deep residual learning for image recognition. In Proceedings of the IEEE conference on computer vision and pattern recognition. 770–778.
[7] Kalvik Jakkala. 2021. Deep Gaussian Processes: A Survey. arXiv:2106.12135 [cs.LG]
[8] Haitao Liu, Yew-Soon Ong, Xiaobo Shen, and Jianfei Cai. 2020. When Gaussian process meets big data: A review of scalable GPs. IEEE transactions on neural networks and learning systems 31, 11 (2020), 4405–4423.
[9] George Y Lu and David W Wong. 2008. An adaptive inverse-distance weighting spatial interpolation technique. Computers & geosciences 34, 9 (2008), 1044–1055.
[10] David JC MacKay et al. 1998. Introduction to Gaussian processes. NATO ASI series F computer and systems sciences 168 (1998), 133–166.
[11] Zeeb B Patel, Palak Purohit, Harsh Patel, Shivam Sahni, and Nipun Batra. 2022. Accurate and Scalable Gaussian Processes for Fine-grained Air Quality Inference. (2022).
[12] Leif E Peterson. 2009. K-nearest neighbor. Scholarpedia 4, 2 (2009), 1883.
[13] Hugh Salimbeni and Marc Deisenroth. 2017. Doubly stochastic variational inference for deep Gaussian processes. Advances in neural information processing systems 30 (2017).
[14] Ryan Sander. 2021. Deep Neural Networks vs. gaussian processes: Similarities, differences, and trade-offs. https://towardsdatascience.com/deep-neural-networks-vs-gaussian-processes-similarities-differences-and-trade-offs-18647376df79
[15] Shan Suthaharan. 2016. Support vector machine. In Machine learning models and algorithms for big data classification. Springer. 207–235.