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Modeling Uncertainty Quantification of NDVI of Agricultural Fields through Bayesian Linear Regression in Time Series Prediction

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ABSTRACT. The current research discusses the applications of Bayesian linear regression to predict the uncertainty of remote sensing data. To predict the uncertainty, the study considered the SENTINEL-2 satellite data of agricultural fields of Uttar Pradesh state of India. Using the stratified sampling method in Google Earth Engine, the random points generated are mapped to agricultural fields. Data was collected in the form of maximum Normalized Difference Vegetation Index (NDVI) values of each agricultural field. The dynamics of the time series predictions were explored with Bayesian linear regression, a probabilistic deep learning method. The model uncertainty defined as epistemic uncertainty is evaluated with the prior and posterior probability parameters of Bayesian statistics in linear regression. The number of regression lines predicted for the same data shows evidence of uncertainty. The Bayesian linear regression models show evidence of high uncertainty for the predicted NDVI values. The variation in model uncertainty is measured by dividing the dataset into samples and it is observed that with increase in data the uncertainty is reduced. Also, with the increase in data, the posterior density becomes sharper which corresponds to a decrease in variance. Further, the study extended the concept of regression analysis with Gaussian basis functions to determine the effect of model uncertainty with an increase in data. The analysis has shown the same result in knowing the effect of uncertainty with the increase in data. Further, a nonlinear polynomial regression model with a Gaussian distribution as a basis function was developed to evaluate the marginal probabilities of the evidence function in capturing the uncertainty with varying degrees of freedom. The polynomial regression with a Gaussian distribution using Bayesian statistics has captured the uncertainty and confirmed that the uncertainty is captured at lower degrees of freedom.

Keywords: SENTINEL-2, epistemic uncertainty, normalized difference vegetation index, bayesian regression, gaussian basis function

1. Introduction

The fundamental goal of remote sensing is to capture information about objects from remote locations. The information generated is not accurate, and there is an element of uncertainty associated with the results obtained from remote sensing techniques. The problem of uncertainty is central in remote sensing and has got relatively modest attention. Uncertainties may arise during acquisition, pre-processing, and from all possible sources from which imperfections could originate. Different degrees of uncertainty arise due to the complexity of the earth's surface, errors in the calibration, the limitations of the radiometric resolution of a sensor, and during processing of remote sensing imagery. Due to uncertainty, when the image is classified, it leads to confusion among pixels belonging to different categories in the image.

The two sources of uncertainty in remote sensing data are spatial distribution uncertainty and semantic uncertainty. The spatial distribution uncertainty arises from the differences in the spatial distribution of different pixels and mostly due to mixed pixels (mixels) in an image. The degree of classification uncertainty is high in mixels and further the uncertainty in the spatial distribution is affected by boundary pixels. Semantic uncertainty in remote sensing data is due to intra-class variability among the pixels. Similar pixels in the image will have the same spectral and spatial features, but spectral features will differ within the image due to noise. Gillmannet et al. (2018) showed that as the spatial resolution increases, the intra-class variability among pixels also increases, thus causing difficulty in image classification and leading to more uncertainty. Objects with diverse internal heterogeneity and higher heterogeneity in the remote sensing image are more likely to be misclassified. These differences will increase the semantic uncertainty between pixels in the image. The quantitative uncertainty description of the image is obtained with object-oriented segmentation performed on relatively homogeneous objects, while the classification uncertainty is measured based on the segmentation results.

The two sources of uncertainty of a deep learning model measured are data uncertainty and model uncertainty. Estimating model uncertainty is more difficult as compared to data uncertainty as it measures uncertainty because of maximum likelihood training on data. Data uncertainty will arise due to noise in the data. Gal and Kendall (2017) demonstrated that aleatoric and epistemic uncertainty are the two main sources of model uncertainty. Aleatoric uncertainty is an inherent property of the data

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distribution, and it is irreducible. Epistemic uncertainty about a deep learning model built with limited data arises due to inadequate knowledge about the system. For data-rich problems, AI-based methods are used to build efficient models, but these data-rich problems are noisy, incongruous, and multimodal. Gal and Kendall (2017) showed that predictive models without uncertainty quantification are inaccurate, and deep learning models incorporating uncetainty quantification are described as well-suited predictive models for the decision-making process.

The uncertainty that needs to be quantified arises from situations like the collection and accuracy of training data, building the deep learning model with limitations, and checking the performance of the model based on operational data. Deep learning architectures and uncertainty quantification are used to build predictive models. These models face at least four groups of problems that overlap: the lack of a theory, the lack of causal models, the sensitivity to imperfect data, and the cost of computing.

2. Modelling Uncertainty Quantification Using Bayesian Techniques

Deep learning methods are successful in solving real-world problems, but researchers do not trust the accuracy and reliability of their predictions. To resolve these issues, Bayesian Deep Learning (BDL) and Bayesian Neural Networks (BNN) are introduced as a bridge between deep learning models and Bayesian statistics. These methods can handle problems with overfitting and are taught to understand how the model parameters work.

2.1. Monte Carlo (MC) Dropout

With the Monte Carlo method, the posterior inference can be computed exactly in deep learning models. But this method is slow and computationally expensive when integrated with deep learning architectures. To compute the prediction uncertainty, the MC method was integrated with dropout as a regularisation term. It is observed that the MC dropout has solved the overfitting problem in deep learning models. Several authors have used dropout to estimate the uncertainty quantity. Wang et al. (2019) have solved medical image segmentation problems using deep convolutional neural networks (CNN) to estimate epistemic and aleatoric uncertainty. They have applied the MC sampling technique to estimate the probability density function of the output segmentation. Liu et al. (2019) have proposed a new unified model for CNN using the stochastic gradient descent method to estimate epistemic and aleatoric uncertainty. Towards this, they used the Bernoulli distribution at the hidden and output layers of neurons with MC dropout. Nair et al. (2019) created a three-dimensional CNN that can segment organ classification problems from MRI sequences and estimate four types of uncertainty. Amini et al. (2018) have computed model uncertainty in BNN with two dropout methods, i.e., Bernoulli dropout and spatial Bernoulli dropout, for end-to-end autonomous vehicle control experiments. Mcclure et al. (2016) used Gaussian dropout to sample the weights and to estimate the uncertainty accurately instead of sampling the weights directly. Using Gaussian dropout and Bernoulli dropout, they have improved the accuracy of CNN architectures and proposed a novel model called the spike-and-slab sample normalization Teye et al. (2018) combined the MC method and Batch normalization process using Bayesian statistics to estimate model uncertainty of the U-Net CNN deep learning model to segment myocardial arterial spin labeling tissues. Yu et al. (2019) developed a semi-supervised learning model to estimate the model normalization with batch normalization in the MC process of segmenting the left atrium from 3D MRI images.

2.2. Comparison of Uncertainty Quantification Methods

Several authors have conducted studies to compare different uncertainty quantification (UQ) models. Foong et al. (2019) estimated the epistemic uncertainty using shallow BNN. They have compared MC dropout and mean-field Gaussian Variational Inference to estimate the epistemic uncertainty. Siddhant et al. (2018) designed various deep learning models using ANN and CNN and applied the MC dropout to estimate and compare the model uncertainty among the various models. Hubschneider et al. (2019) used MC dropout and the bootstrapping ensemble technique to estimate and compare model uncertainty in the task of vehicle control. Mukhoti et al. (2018) designed several deep-learning models and estimated model uncertainty using MC dropout in regression problems.

2.3. Variational Inference

Variational Inference (VI) is an approximation method built with prior and posterior distribution parameters over BNN weights to estimate the model uncertainty. To model uncertainty, Bayesian inference is viewed as an optimization problem that can be used to train deep neural networks (DNN) using the stochastic gradient descent method (SGD). Posch et al. (2019) estimated the posterior distribution uncertainty of the DNN using the product of probability density parameters of Gaussian distributions with eigenvalues of covariance matrices. Krishnan et al. (2019) used deterministic weights from a pre-trained DNN to estimate the model uncertainty with a transfer learning mechanism. Subedar et al. (2019) addressed epistemic uncertainty using a multimodal Bayesian fusion framework for human activity recognition. Marino et al. (2018) estimated model uncertainty for deep BNN using the SGD method. Louizoset et al. (2017) estimated the model uncertainty with posterior distributions over the weights of neural networks using the SGD variational inference method. Hubin and Storvik (2019) proposed the SGD to estimate model uncertainty through stochastic variational inference. Liu et al. (2020) estimated the probability prediction of uncertainty by integrating variational inference in spatial-temporal neural networks. Ryu et al. (2019) estimated model uncertainty by integrating a graph CNN with the BNN framework. Swiatkowski et al. (2020) improved the signal-to-noise ratio by decomposing the variational parameters into low-rank factorization with Gaussian mean-field variational inference and the SGD method. Farquhar et al. (2020) proposed a deeper linear mean-field network for a shallow full covariance network to estimate model uncertainty.

2.4. Model Uncertainty in Remote Sensing

In the field of remote sensing, most of the work related to data and model uncertainty is done with the semantic segmentation of RADARSAT SAR images. Rottmann et al. (2019) Deep Lab model with MC dropout used Cityscape data to estimate the model uncertainty and obtained an accuracy of 95.3% and Intersection over Union (IoU) of 78%. They have developed uncertainty graphs for predictive entropy and mutual information to predict pixel uncertainty. Kendall et al. (2015) applied MC dropout in the SegNetCNN architecture on CamVid Road Scenes and SUN RGB-D Indoor Scene datasets. They compared different neural network architectures to the SegNet architecture and made aleatoric and epistemic uncertainty maps for all classes and for each class using K-fold cross-validation mechanisms. Huang et al. (2018) proposed a method of "concrete dropout" by modifying the traditional "MC dropout" to improve the accuracy of SegNet architecture. LaBonte et al. (2019) compared MC dropout to the BDL Model by sampling weights from the posterior distribution. The BDL model learns the prior and posterior parameters of the distribution instead of the weights, and it is observed that the model produces better accuracy after training the data for several times. The Bayesian parameters have produced interpretable uncertainty maps to compare the differences in uncertainty. CNN architectures for high-resolution image semantic segmentation were proposed by Kampffmeye et al. (2016). They have removed uncertain pixels from prediction, and uncertainty maps are designed using MC dropout. They showed improvement in accuracy from 90 to 97.5%. Haas and Rabus (2021) have applied deep learning techniques to RADARSAT SAR images for semi-automated road segmentation. The deep learning framework developed with MC dropout is used to develop uncertainty maps and for the classification process to improve accuracy.

With this background, it is observed that there is a need to explore the model uncertainty for time series data in remote sensing images. To explore model uncertainty, a time series prediction model was developed for SENTINEL-2 NDVI (Normalized Difference Vegetation Index) using Bayesian Linear Regression and estimated the model uncertainty with Bayesian Parameters as mentioned above.

2.5. Normalized Difference Vegetation Index (NDVI)

Researchers and scientists use the NDVI as a standard tool to assess vegetation cover, plant growth, crop phenology, and biomass production using multispectral satellite data. Over the past few years, many NDVI products have been made from different sensors data. These products can be used for quantitative and qualitative analysis of time series predictions. The NDVI describes the health and greenness of different vegetation conditions considering the difference between near-infrared (which vegetation strongly reflects) and red light (which vegetation absorbs). The NDVI vary from –1 to 1. In satellite data, objects like cloud, shadows are represented with more than the value 1, water bodies as –1, and 0 for no vegetation cover. The NDVI values between 0.8 and 0.9 indicate greater densities of green leaves while the values from 0.2 to 0.5 for shrubs and grasslands or senescing crops. Healthy vegetation has a high chlorophyll content, reflecting more in near-infrared (NIR) and green light whereas unhealthy vegetation reflects less NIR. Similarly, when the plant reaches a greener stage, it will have a higher reflectance of NIR than when it is growing in different stages, providing distinct signal values to identify the growth cycle of a plant. The NDVI is given as:

$$NDVI = \frac{NIR - R}{NIR + R} \tag{1}$$

where *NIR* stands for near-infrared, and *R* stands for red light from the visible spectrum.

3. Data and Methodology

Uttar Pradesh is the largest state in the Indo-Gangetic Plain, producing wheat and rice every year. To explore the time series prediction dynamics using Bayesian linear regression, the study considered the SENTINEL-2 product of the whole Uttar Pradesh state, India. The SENTINEL-2 images are collected and pre-processed with less than 5% cloud cover using the Google Earth Engine, for the period from January 1 to December 31, 2021. The NDVI was derived from the red (Band 4) and near-infrared (Band 8) spectral bands with spatial resolutions of 10 m of SENTINEL-2 datasets. The study generated 100 random points, imposing the criteria that they should be over farmland growing a certain crop. To achieve this, the study used GFSAD1000 (Cropland Extent 1 km, Crop Dominance, Global Food-Support Analysis Data) from the Google Earth Engine (GEE) CatLog to select the pixels that are farmland growing wheat and rice. The stratified sample method in GEE CatLog allows mapping the random points on the pixels, which are agricultural fields. The agricultural fields mapped are shown in Figure 1. The study used a maximum NDVI value for each crop collected from 100 agricultural fields and evaluated for uncertainty. The study considered the entire 2021 dataset to build the deep learning model for time series prediction. The distribution of NDVI values is shown in Figure 2.

Bayesian Linear Regression: Linear regression models are linear with explicit parameters but not with their input variables. Linear models can model non-linearity from input variables to targets like in polynomial regression. In general, a linear regression can be written as:

$$y(x, w) = w^T \varphi(x) \tag{2}$$

The target variable t of an observation x is provided with a deterministic function $y(x, w)$ and random noise ε:

$$t = y(x, w) + \varepsilon \tag{3}$$

The study assumed that the noise is normally distributed with zero mean and variance one, and the corresponding probabilistic model is:

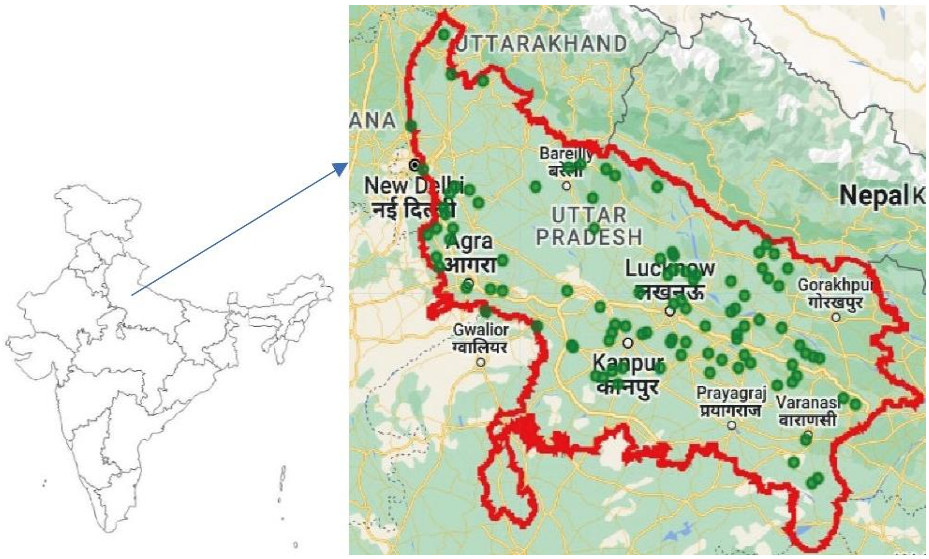

Figure 1. Location of the agricultural fields selected for the study.

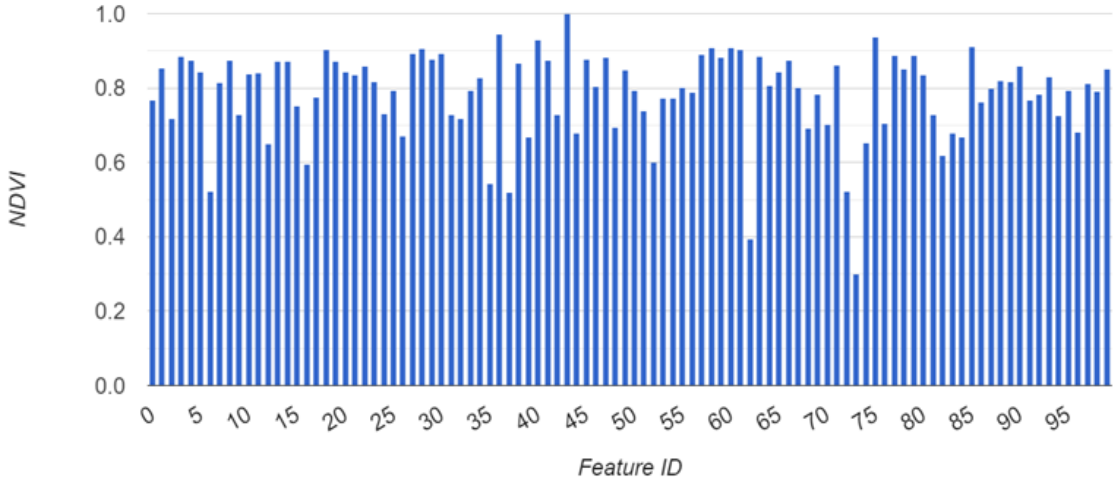

Figure 2. Maximum NDVI of 100 agricultural fields for year 2021.

$$p(t/X,w,\beta)=\prod_1^N N\left(\frac{t_i}{w^T}\varphi(x),\beta^{-1}\right) \tag{4}$$

To fit the model and for inference of model parameters, training set of N independent and identical observations x_1, x_2, …, x_N and their corresponding targets t_1, t_2, …, t_N. The sum of squares error function derived from the exponent of the likelihood function is:

$$E_D(w)=\frac{1}{2}\sum_1^N\left(t_i-W^T\varphi(x_i)\right) \tag{5}$$

where $\varphi(x_i)$ is the design matrix.

To define the Bayesian linear regression, there is a need for prior probability distribution over model parameters w. The probability distribution is a Gaussian distribution over model parameters w with zero means:

$$p\left(\frac{w}{\alpha}\right)=N\left(\frac{w}{o},\alpha^{-1}I\right) \tag{6}$$

The posterior distribution built with the log-likelihood prior probabilities is given as:

$$\log p\left(\frac{w}{t},\alpha,\beta\right)=-\beta E_D(w)+constant \tag{7}$$

where $E_D(w)=\frac{1}{2}w^Tw$.

The parameters α and β are obtained by maximizing the integral of likelihood:

$$w\cdot\left(\frac{t}{\alpha},\beta\right)=\int p\left(\frac{t}{w},\beta\right)p\left(\frac{w}{\alpha}\right)dw \tag{8}$$

Maximizing the above equation will result in marginal likelihood concerning the parameters α and β. The mean and standard deviation of these distributions are used to calculate epistemic uncertainty.

Once the data was obtained, the prior and posterior probabilities of the samples were evaluated. The distribution defined is the Gaussian distribution and is distributed over the model parameters as described in Section 3.2. Bayesian linear regression is defined with the model parameters, and the probability of the predictions is shown in Figure 3. As the noise is removed, we are interested in model uncertainty. The model uncertainty, i.e., epistemic uncertainty defined in terms of mean and standard deviation, will lie in that range. The model uncertainty evaluated is shown in Figure 3.

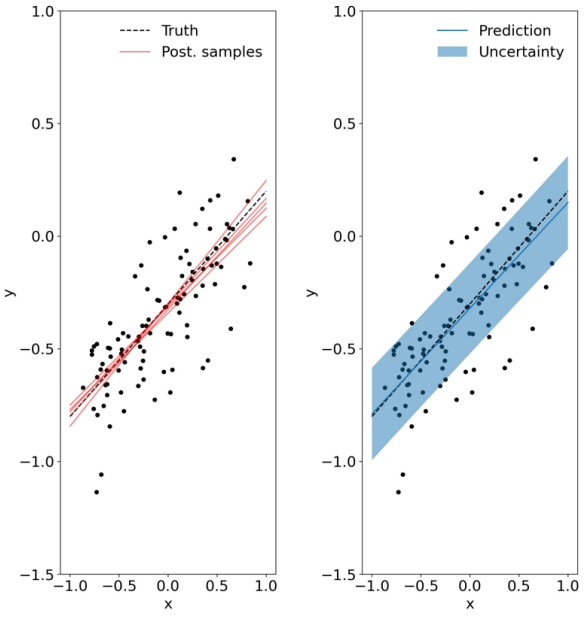

Figure 3. Epistemic uncertainty of NDVI data.

4. Results and Discussion

4.1. Machine Learning Approaches in Modeling Uncertainty

The spatiotemporal process became a strong candidate for many machine learning methods because of its complex interactions and high dimensionality. While there is numerous machine learning and deep learning models for nonlinear spatiotemporal processes, the explicit dynamics of these processes remain unexplored. Though feed-forward neural networks model the multi-variate processes, they are not designed to capture dynamic time-sequential interactions between the variables. Several researchers tried to explore the dynamics of the spatiotemporal process, but Recurrent Neural Networks (RNN) proved to be a potential model to explore the nonlinear dynamics in multivariate sequential systems. However, RNN suffered from a "vanishing gradient" problem and made these models difficult to estimate the backpropagation parameters in the spatiotemporal process. But RNNs have been increasingly used to model complicated forecasting problems such as visual object tracking, speech recognition, and text generation. RNN replicates complex attractor dynamics in chaotic systems and is considered a black box method for capturing complex sequential relationships between the variables for modeling dynamic problems. RNNs are referred to as echostate networks which randomly simulate the parameters of the hidden state of backpropagation, thereby reducing it to a regression problem.

Deep learning tools like ANN, and CNN dropout representing model uncertainty is of crucial importance to address the issue. With the introduction of Bayesian uncertainty, new deep-learning models have evolved. Standard deep learning regression and classification models do not capture epistemic uncertainty. In classification and regression models the predictive probabilities with SoftMax output are represented as model confidence and they are uncertain in nature. An agent in reinforcement learning can decide when to exploit and when to explore uncertain information. An agent in reinforcement learning will learn much faster with uncertainty estimates over Q-valued functions and techniques like Thomson sampling.

Bayesian probability theory is a mathematical approach to model uncertainty but is computationally expensive as compared to other mathematical models. To avoid this computational cost dropout and its variants are considered as Bayesian approximation and designed as a probabilistic model. This dropout approximation "integrates over the models" weights as a Gaussian process. Finite Neural Networks with Gaussian distributions over the weights have been studied as BNN to model uncertainty in DNN architectures. Another method to model the uncertainty is "variational inference" in BNN but with limited success which offers robustness in overfitting. Recent advances in variational inference are "sampling-based variational inference" and "stochastic variational inference" to model the uncertainty, but these models come with a prohibitive computational cost. As compared to the dropout technique, variational inference requires more parameters (double the size) for the same network size and more time to converge to the Gaussian process. To overcome the difficulty, "expectation propagation" in hidden layers is introduced to reduce the Root Mean Square Error (RMSE).

4.2. Observations from the Current Study

In Figure 3 the x-axis represents NDVI values, and the corresponding regression values are represented on the y-axis. From Figure 3, it is observed that for the same data, the Bayesian linear regression model shows a greater number of regression lines, which signifies that the epistemic uncertainty is high for the model built on this data. The shaded region is the epistemic uncertainty, and it shows that the error lies in that region for each point predicted with Bayesian statistics. Further, to know the variations in uncertainty, the dataset is divided into three subsets of sizes 20, 50, and 70. The data is normalised with a normal distribution in the range [–1, 1]. This process is done to show that as the data size increases, epistemic uncertainty is reduced. The results are shown in Figures 4 to 6.

Figures 4 to 6 show the number of regression lines (red colour) for the random weight samples drawn from the posterior distribution. The true parameters of the regression line are plot-

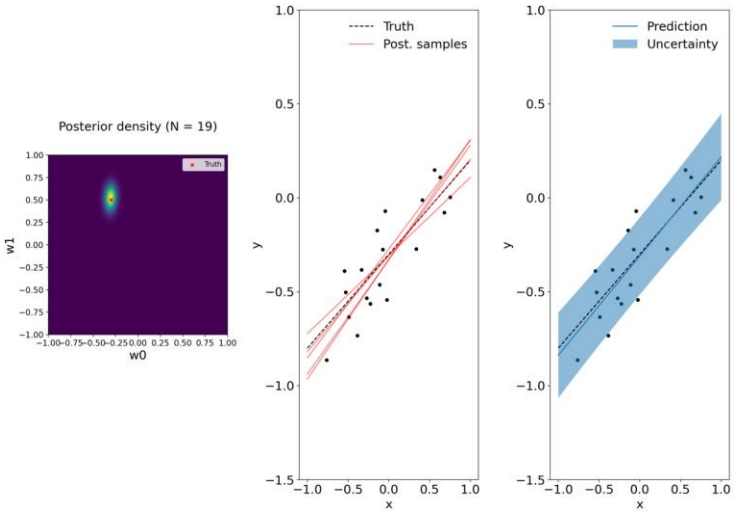

Figure 4. Epistemic uncertainty with 20 samples.

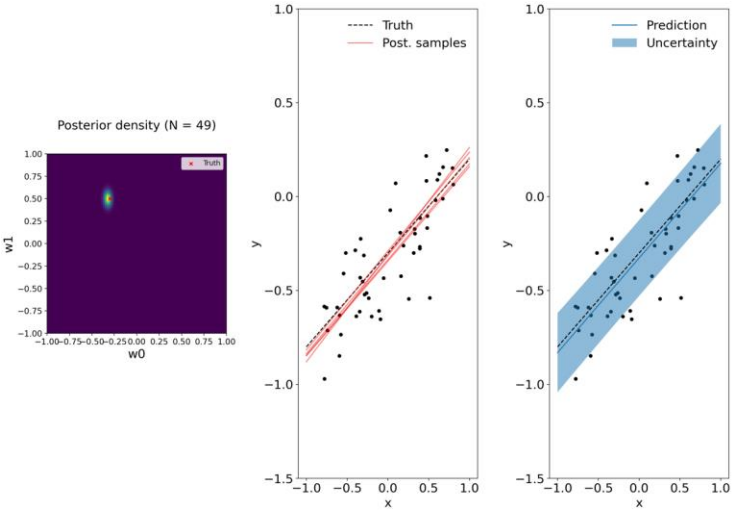

Figure 5. Epistemic uncertainty with 50 samples.

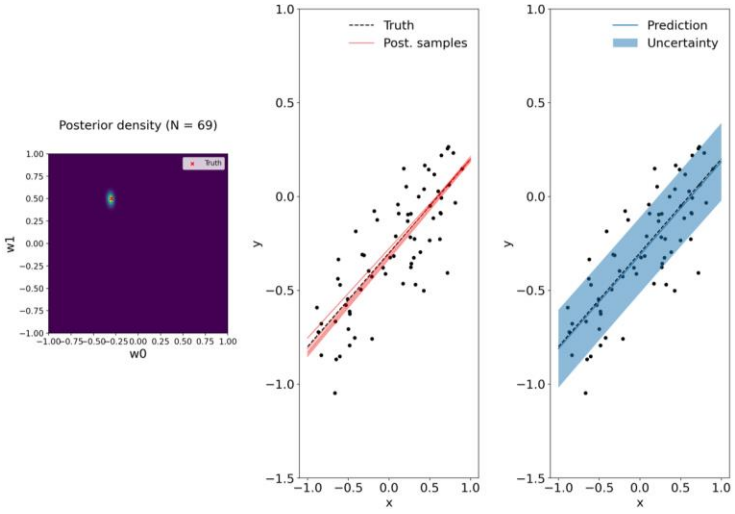

Figure 6. Epistemic uncertainty with 70 samples.

ted as a dashed black line, and the training data with Gaussian noise embedded is plotted as black dots. Figure 4 shows that as the number of data points goes up, the peak of the posterior density gets sharper. This is the same as the variance of random samples going down in the second column and the epistemic uncertainty going down in the third column.

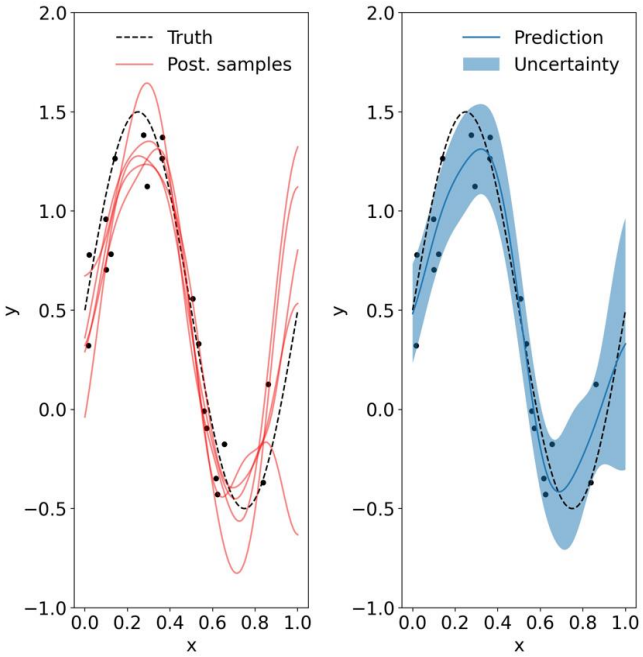

Figure 7. Epistemic uncertainty with 20 samples using Gaussian basis functions.

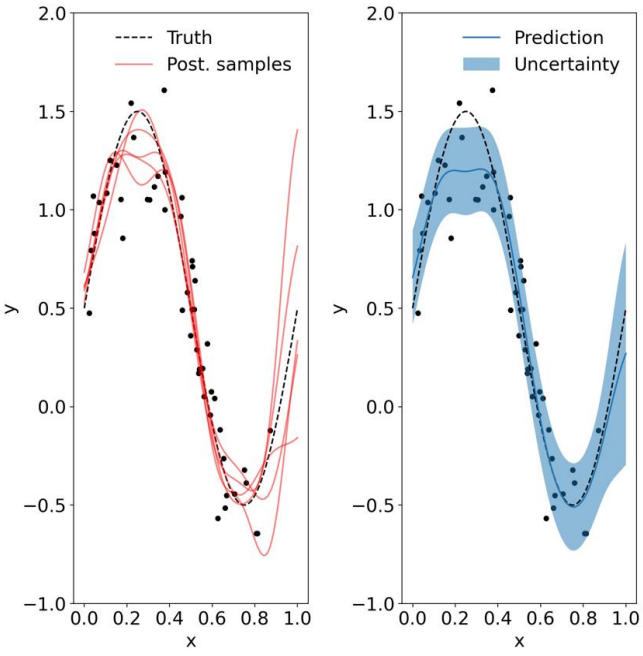

Figure 8. Epistemic uncertainty with 50 samples using Gaussian basis functions.

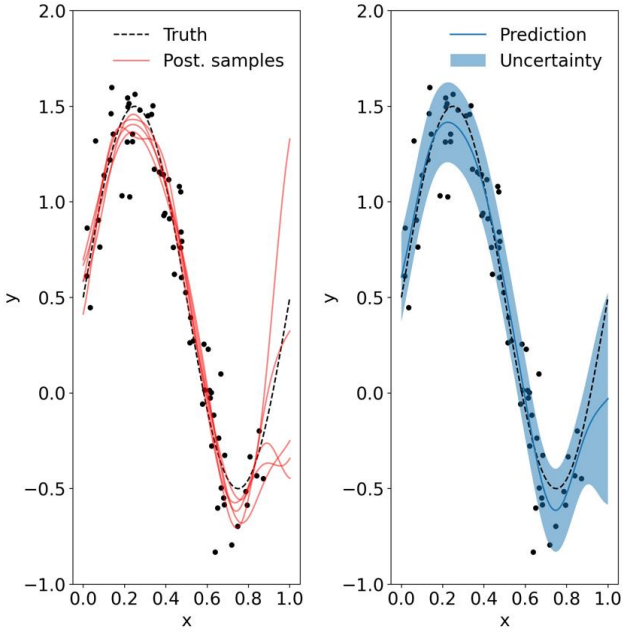

Figure 9. Epistemic uncertainty with 70 samples using Gaussian basis functions.

Further, the study extended the concept of Bayesian regression analysis with Gaussian basis functions of mean 0 and variance 1. From Figures 7 to 9, it is observed that the posterior variance and the prediction uncertainty of the samples drawn decrease with an increase in data, and it shows that the epistemic uncertainty is high with fewer samples.

Moreover, a nonlinear regression model (polynomial regression) is built with varying degrees of freedom to capture the epistemic uncertainty. For evidence function, we have chosen ten polynomial basis functions of varying degrees. The polynomial regression with Gaussian distribution using Bayesian statistics defined with marginal probabilities of the evidence function is shown in Figure 10. It is observed that the polynomial regression with degree 4 only has captured the epistemic uncertainty and there is no difference with the polynomials of the highest degree in comparison. The polynomial regression model with higher degrees of freedom is not needed to capture the uncertainty as data is sufficiently embedded in the shaded region of regression model with degree 4 and confirms that marginal likelihood evaluation favours models of intermediate complexity.

5. Conclusions

In this work, we have assessed the epistemic uncertainty of the remote sensing data with probabilistic deep learning techniques. The study considered the Bayesian Linear Regression technique as a probabilistic deep learning model to estimate the model uncertainty. To make the analysis of the deep learning model built with remote sensing data, we have considered GFSAD1000 and SENTINEL-2 NDVI time series data of wheat and rice agricultural fields of Uttar Pradesh state in

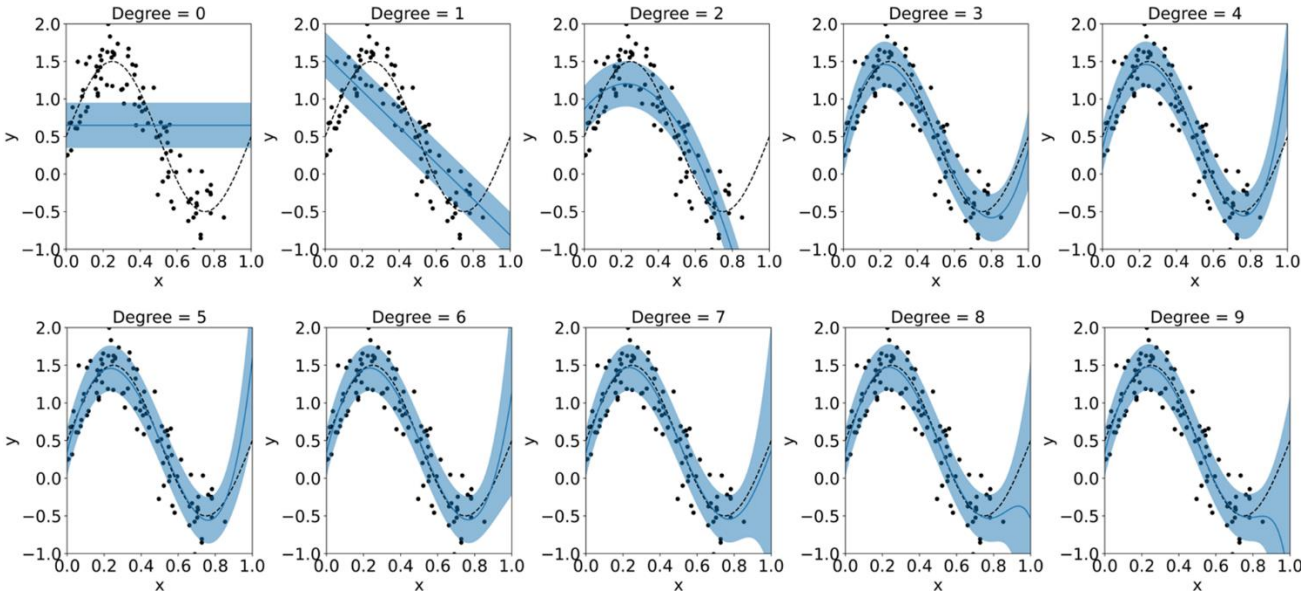

Figure 10. Polynomial regression with varying degrees of freedom.

India. The results of the regression model showed a decrease in epistemic uncertainty with an increase in data size. It is observed that the posterior density gets sharper with an increase in data size. The Bayesian Linear regression model did not capture the uncertainty for all the data points. To capture the uncertainty for all the data points, we have extended the work with Gaussian basis functions. The Gaussian Basis function is added to the Bayesian Linear Regression model and modified Bayesian Linear Regression model as a non-linear regression model to capture the model uncertainty. It is observed that the nonlinear regression model has captured the uncertainty for all the samples of different sizes with less deviation compared to linear regression model. The non-linear regression model developed has shown the same results that the epistemic uncertainty is decreased with an increase in data size. Further, to improve the results, we have designed polynomial regression model with varying degrees of freedom to capture the model uncertainty. The study found that the polynomial regression with the lowest degree captured the uncertainty and there is no difference between the polynomials with the highest degree in capturing the uncertainty. The polynomial regression model with higher degrees of freedom is not required because the data is sufficiently embedded in the shaded region of the regression model with a minimal degree.

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