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Uncertainty Analysis in Machine Learning Models

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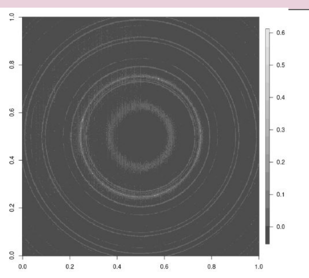
1. INTRODUCTION

- **Background of the Study:**
- Machine Learning (ML) Models are increasingly being used in Science and Engineering
- A lot of studies on ML models focus on improving predictive power of ML models
- Another vast area of consideration is quantifying the uncertainties (epistemic(reducible)/aleatory(irreducible)[1]) surrounding these prediction
- **Motivation of the Study:**
- ML models struggles with Out-Of-Distribution (OOD)[2] samples, especially those from complex data set.
- Prediction uncertainty increases with increase in opacity of ML models
- **Goal of the Study:**
- Quantify uncertainties surrounding the prediction of β-phase volume fraction in a Ti-6Al-4V alloy[3] by features of its 2D diffraction images using Gaussian Process Regression (GPR) and Convolution Neural Networks (CNN)

2. METHODOLOGY

Approach I (CNN)

Ingest 2D diffraction images Data set



2048 X 2048

Hyper-Parameters Tuning for CNN

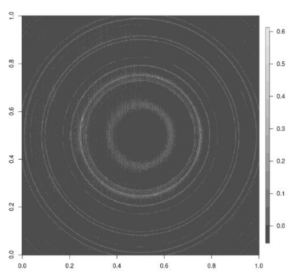
Well-tuned Hyper-parameters include:
- Number of conv. layers
- Number of max-pooling layers
- Node numbers in each layer
- Dropout layer
- Regularization
- Normalization

Quantify the Uncertainty of the analysis

Best performance model's structure will be chosen to do uncertainty quantification.
- The model is trained 100 times with different initial values to observe its final convergence results

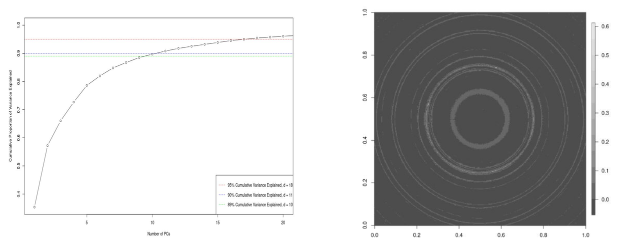
Approach II (GPR)

Ingest 2D diffraction images Data set



2048 X 2048

Reconstruct the data set based on determined number of PCs



Reconstructed 2D diffraction images

PCA is employed here as a dimension reduction technique reduce computational cost

Model relationship between chosen PCs and β-phase volume fraction using GPR

- GPR as a non-parametric regression model provides probability distribution over functional relationships
- It models the relationships using the mean and kernel function
- GPR is used to both make predictions and quantify the uncertainty associated with the predictions

Let $S = \{(x^{(i)}, y^{(i)})\}_{i=1}^{m}$ be a training set, the **GPR model** is given as $y^{(i)} = h(x^{(i)}) + \epsilon^{(i)}, \quad i = 1, \ldots, m$ where $h(\cdot) \sim \mathcal{GP}(m(\cdot), k(\cdot,\cdot))$ and

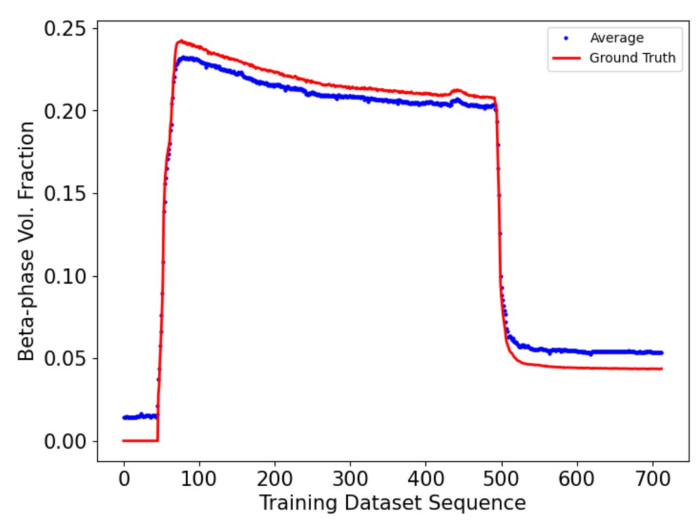
$$(m(\cdot), k(\cdot,\cdot)) = \left(\begin{bmatrix} m(x_1) \\ \vdots \\ m(x_m) \end{bmatrix}, \begin{bmatrix} k(x_1,x_1) & \cdots & k(x_1,x_m) \\ \vdots & \ddots & \vdots \\ k(x_m,x_1) & \cdots & k(x_m,x_m) \end{bmatrix} \right)$$

$$k(x_i,x_j) = \sigma^2 \exp\left(\frac{-|x_i - x_j|^2}{\beta} \right), \ \epsilon \sim \mathcal{N}(0, \delta^2)$$

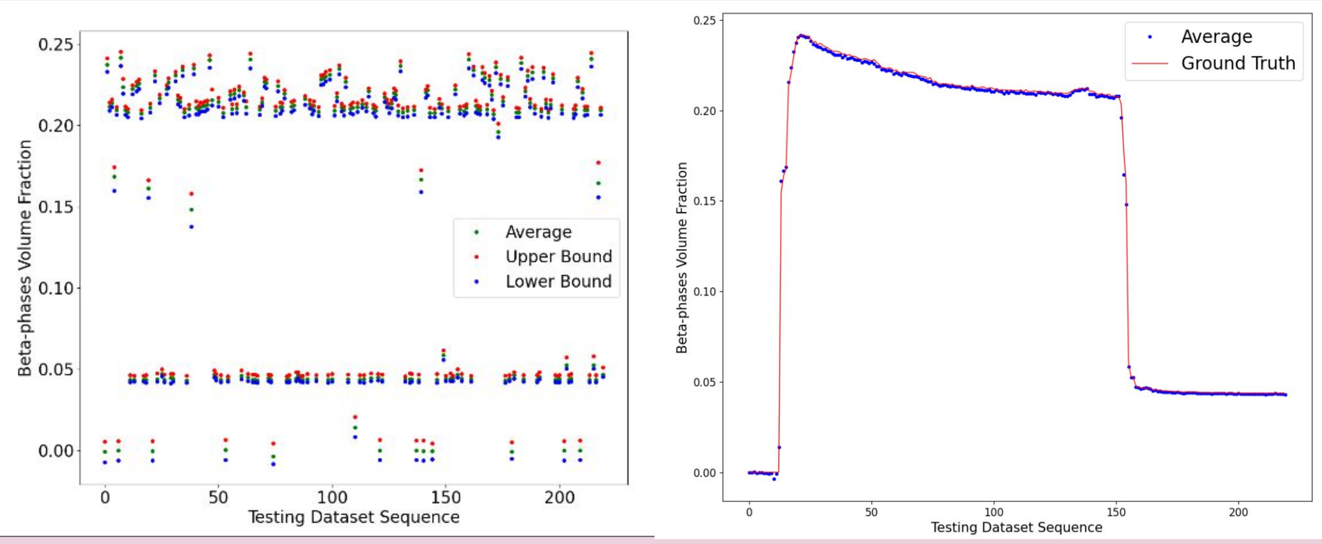
Quantify the Uncertainty of the analysis

3. RESULTS

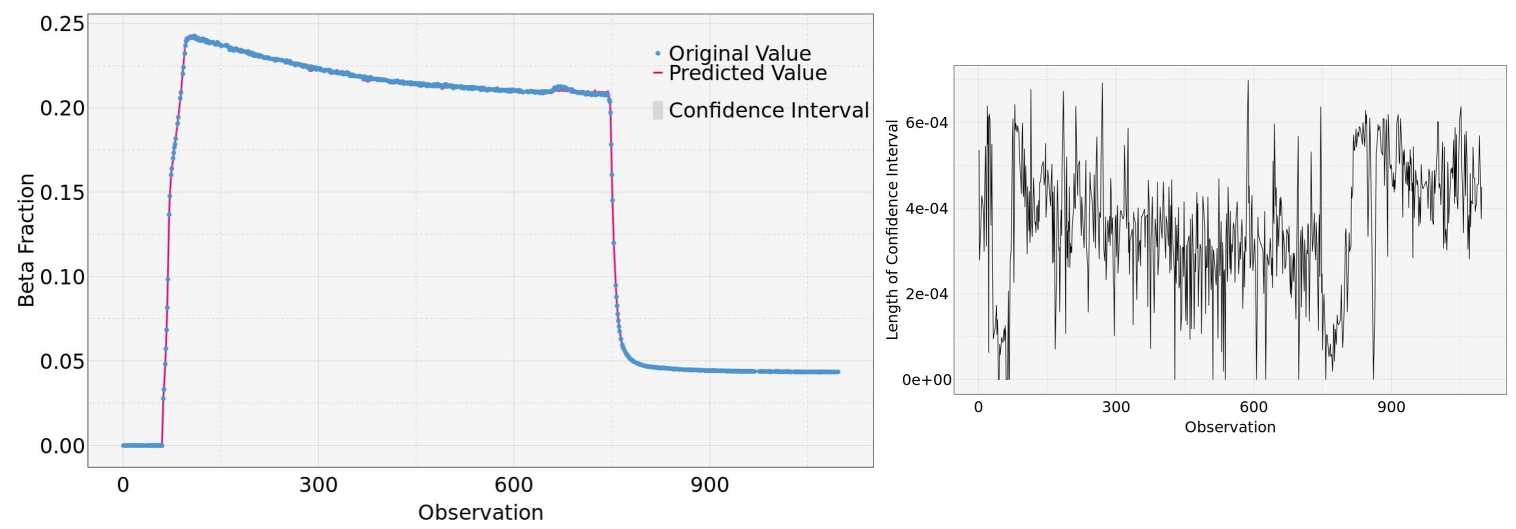
```
Layer (type)                  Output Shape              Param #
=================================================================
input_2 (InputLayer)          [(None, 2048, 2048, 1)]   0

conv2d_5 (Conv2D)             (None, 2046, 2046, 16)    160

max_pooling2d_5 (MaxPooling    (None, 1023, 1023, 16)   0
2D)

conv2d_6 (Conv2D)             (None, 1021, 1021, 32)    4640

max_pooling2d_6 (MaxPooling    (None, 510, 510, 32)     0
2D)

conv2d_7 (Conv2D)             (None, 508, 508, 64)      18496

max_pooling2d_7 (MaxPooling    (None, 254, 254, 64)     0
2D)

conv2d_8 (Conv2D)             (None, 252, 252, 128)     73856

max_pooling2d_8 (MaxPooling    (None, 126, 126, 128)    0
2D)

conv2d_9 (Conv2D)             (None, 124, 124, 256)     295168

max_pooling2d_9 (MaxPooling    (None, 62, 62, 256)      0
2D)

flatten_1 (Flatten)           (None, 984064)            0

dense_2 (Dense)               (None, 128)               125960320

dense_3 (Dense)               (None, 1)                 129

=================================================================
Total params: 126,352,769
Trainable params: 126,352,769
Non-trainable params: 0
```



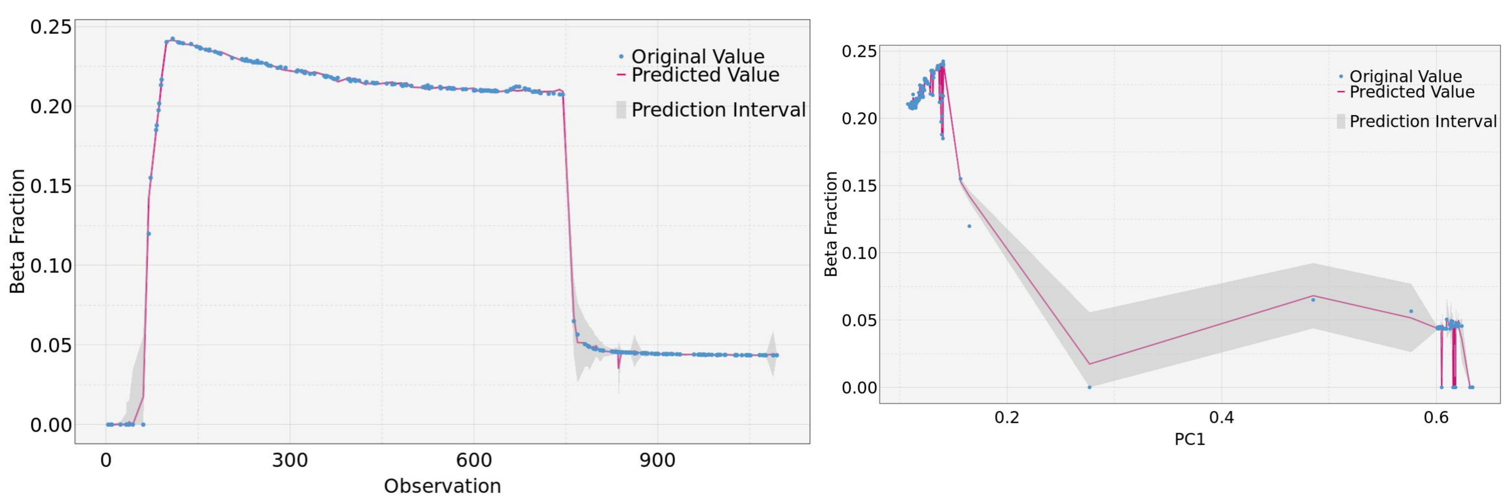
(left): Architecture of the CNN model trained 100 times. (right): CNN model's average predicted results. The red line represents the ground truth, while the blue plots depict the average predicted results. The MSE in this case is 3.47e-06



CNN model; (left): shows average predicted values (green dots), maximum predicted values (red dots), and minimum predicted values (blue dots) for each of the testing set. (right): shows the ground truth (black dots), upper bound of the predicted result (red line), and lower bound of the predicted results (blues line) for each data point in the testing set



(left): Original vs. Predicted β-fraction with 95% confidence interval for train set using GPR.
(right): Length of the 95% confidence interval for train set.



(left): Original vs. Predicted β-fraction with 95% prediction interval for test set using GPR.
(right): Original vs. Predicted β-fraction with corresponding 95% prediction interval for PC1

Set	Sample size(n)	%	Train (Time)	Train (MSPE)	Test (MSPE)
I	1056	95	40 min 30 sec	2.8402e-09	2.5566e-06
II	1097	95	12 min 16 sec	4.4114e-07	4.9103e-06
III	855	95	-	-	-
IV	3008	95	-	-	-
III	855	90	1 hrs 59 min 15 sec	1.9824e-11	3.7309e-04
IV	3008	90	-	-	-
IV	3008	83	6 hrs 26 min 48 sec	1.3631e-07	2.6590e-05

- % represents the percentage of the variations in the diffraction images for each data set explained by the chosen number of PCs.
- We leveraged on HPC values for the modelling and the training time recorded were obtained using 10 cores

4. CURRENT CHALLENGES

Data Set	Sample Size (n)	# PCs (d)	# PCs (d)
I	1056	5, <u>7</u>	22
II	1097	<u>5</u>, 7	22
III	855	5, 7, 10	<u>18</u>, 22
IV	3008	5, 7	<u>22</u>

- There are 4 data sets of different sample sizes
- The first set of Number of PCs are estimable using the current methodology of GPR
- The last set of PCs are inestimable using the current methodology of GPR
- The underlined number of PCs explained 95% of variation in the β-phase volume fraction

The Challenge

- Increase in sample size (n) and feature space (d) increases the computational cost because of:
  - Estimation of correlation matrix
  - Inversion of kernel function
- Current methodology does not allow for parallelization during model estimation

5. SOLUTIONS EXPLORED

- Combine PCA with algorithms that allow for parallelization (i.e. Vecchia Approximation) to extend GPR computation to higher dimensional space and sample size
- Explore various covariance functions to reduce the computational complexity and time taken in the new algorithms to be explored

6. CONCLUSIONS

Performed Uncertainty Quantification for the prediction of β-phase volume fraction using two different approaches

- For data set II:
- CNN which captured the uncertainty of the optimizer has MSE (3.49e-06 (average)) and longer training time (round 6 minutes for each training iteration) x 100 = 10 hours
- GPR has MSE (4.91e-06) and shorter training time (round 12 minutes 16 seconds)

7. FUTURE DIRECTION

- Extend to incorporate methodologies that facilitate uncertainty analysis in ML models with higher feature space and sample size and shorter computational time
- Extend to incorporate methodologies that facilitate uncertainty analysis in ML models in a federated learning environment

8. REFERENCES

[1] Der Kiureghian, A. & Ditlevsen, O. Aleatory or epistemic? Does it matter? *Struct. Safety* **31,** 105-112 (2009)
[2] Nemani, V. *et al.*: Uncertainty quantification in machine learning for engineering design and health prognostics: A tutorial. *Mech. Syst. Signal Process.* **205,** 110796 (2023)
[3] Brown, D. W., *et al.* Evolution of the microstructure of laser powder bed fusion Ti-6Al-4V during post-build heat treatment. *Metallurgical and Materials Transactions* A 52 (2021): 5165-5181

9. ACKNOWLEDGEMENT

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