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A Surrogate Model's Decision Tree Method Evaluation for Uncertainty Quantification on a Finite Element Structure via a Fuzzy-Random Approach

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Abstract

A novel additive manufacturing method (AM)) constructs a three-dimensional model from a computer-aided design by adding material layer by layer. This technique produces a lightweight end product with complex geometries and has gained recognition among industrial players. Nonetheless, the mechanical properties and geometry components are the uncertainties that prevail in its structures. An alternative approach using the Finite Element Method (FEM) to analyse these uncertainties demands extensive computational effort and time consumption. Therefore, a machine learning (ML) tool using the surrogate modelling technique offers an alternative way to provide and predict simulation outcomes. This study applies two surrogate modelling approaches, the decision tree (DT) and the Gaussian process regression (GPR) methods. Output data from a FEM simulation with uncertainty elements are obtained for the training purposes of the surrogate models. Both ML methods can predict simulation results with high precision. Both approaches obtained an excellent coefficient of determination value, R^2 of 0.998, and Root Mean Square Error, RMSE of 0.012, successfully reducing time consumption and computational effort. The DT method shows better robustness when compared to the GPR method. A value change in the input parameter significantly impacts the surrogate model's prediction performance. An adequate quantity of data input for the training phase of both surrogate models exhibits the FEM results with the presence of uncertainty and robustness.

Keywords*: *decision tree; finite element method; gaussian process regression; machine learning; surrogate model; uncertainty analysis

1. Introduction

The advancement of the manufacturing industry has led to the discovery of new technology, such as the additive manufacturing (AM) method. This revolutionary technology produces less waste and lightweight materials during the manufacturing process. Moreover, this recent manufacturing method can have complex components from computer-aided design (CAD) drawings to end products. Besides, it consumes less energy regarding tooling and workers' perspectives (Seharing et al., 2020). Thus, it has gained the attention of crucial industrial players, especially in the research and development sector. However, further research has discovered specific variability in the end-product quality, proving that uncertainties exist. Mahadevan et al., (2022) have highlighted that those uncertainty factors might occur because of porosity in the AM product microstructure, material properties, and residual strength created during the manufacturing process.

Researchers have Identified a few scientific methods to overcome these issues, for example, by conducting physical experiments to analyze these uncertainties. However, extensive waste has been created due to consumable materials, sample disposal, and failed experiments. Therefore, another alternative method is by implementing computational approaches, such as the Finite Element Method (FEM). Nonetheless, specific FEM simulations are related to a multi-physics basis and require complex modelling, and it requires a further computational approach, increased cost, and more simulation time run. Emerging research nowadays has discovered Artificial Intelligence (AI) technology which is linked to a machine learning (ML) tool, the surrogate model, as a possible alternative computational method to the FEM simulation. This method can cater to complex and multi-physic models in a lighter approach and steps up simulation to shorten the simulation time (Yan et al., 2020).

In recent years, machine learning tools via surrogate models have been a research subject in vast domains and engineering problems. Figure 1 shows the increasing trend of research publications on surrogate models and machine learning over the last five years. Yu et al., (2023) have applied a surrogate optimization model to reduce the finite element calculation and shorten the time consumption. Meanwhile, Perera et al., (2020) have implemented the neural network method to identify damage on a large complex 3D finite element model. Wang et al., (2022) monitored the structural health of a concrete bridge using the Gaussian process regression (GPR) method and finite element model updating.

Furthermore, Arabbeiki et al., (2023) have conducted research on a finite element model of a bone segment using the DT method. Xia et al., (2021) have shown a Computational Fluid Dynamics (CFD) simulation under uncertain conditions to evaluate the efficiency of a surrogate model. Abid et al., (2020) have carried out an uncertainty analysis on shape memory alloy microactuators by combining the finite element method, surrogate model, and Monte Carlo simulation. Therefore, this study uses the surrogate model approach to incorporate uncertainty parameters in a FEM.

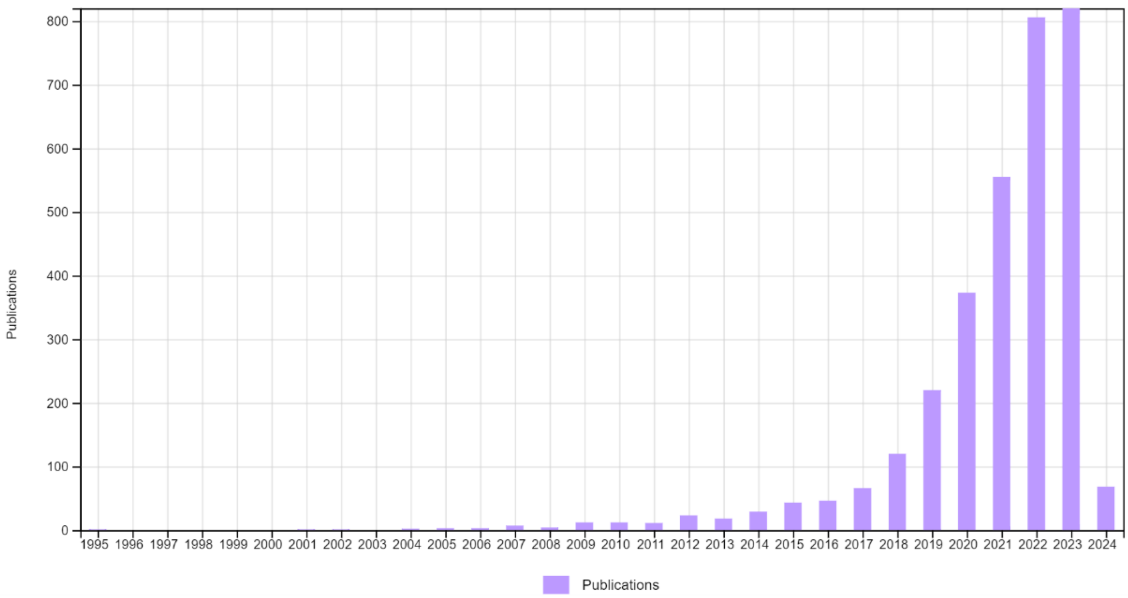


Figure 1 Research trend of surrogate models and machine learning based on publications: adapted from Web of Science (2024)

2. Objectives

A rectangular-shaped and hollow steel plate was created as the FEM study case. Axial loading and other boundary conditions were applied to the plate. The FEM output analyzed in this paper is the von-Mises stress (VM) and the displacement of the plate. Based on the previous research above, the specific objectives of this paper are given below.

- To implement uncertainty elements and approaches on the input parameters of the FEM simulation.
- To evaluate the prediction performance of surrogate models, the GPR and DT methods, and compare with the results of a FEM simulation.
- To test the robustness of the prediction performance of the surrogate models in uncertain conditions

3. Methodology

3.1 FEM Model and mesh convergence study

A quarter model of a steel plate was created for modelling purposes. Figure 2 illustrates the plate model with its boundary condition and dimension. An equally distributed force was implemented on top of the steel plate. The figure also shows the angle direction of the quarter-hole part of the model. For simulation works, the angle φ is defined as 90°. The plate is meshed using triangular-shaped elements. Seven meshed models, Model I, II, III, IV, V, VI, and VII, which have different numbers of nodes and elements, were created for the mesh convergence study. Each model was subjected to a stress simulation study, and the mesh convergence was obtained when the graph curve acquired a stable condition at 16 MPa of stress value, as presented in Figure 3. FEM model VI is chosen for this paper's study as it has already achieved the 16 MPa convergence limit. As represented in Figure 4, the model consists of 180 nodes and 304 elements and is the optimum number of nodes and components for the FEM simulation purposes. Figure 5 shows the flow of each task in this study. Each task is separated into three stages. The FEM simulation is performed, and the output is produced in the first stage. The FEM output is used as the input of the surrogate modelling training and testing phase in the second stage. The last stage is predicting and validating the surrogate models' output.

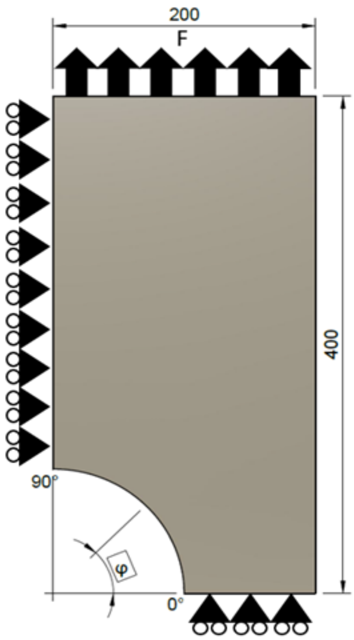


Figure 2 Quarter steel plate model with angle orientation

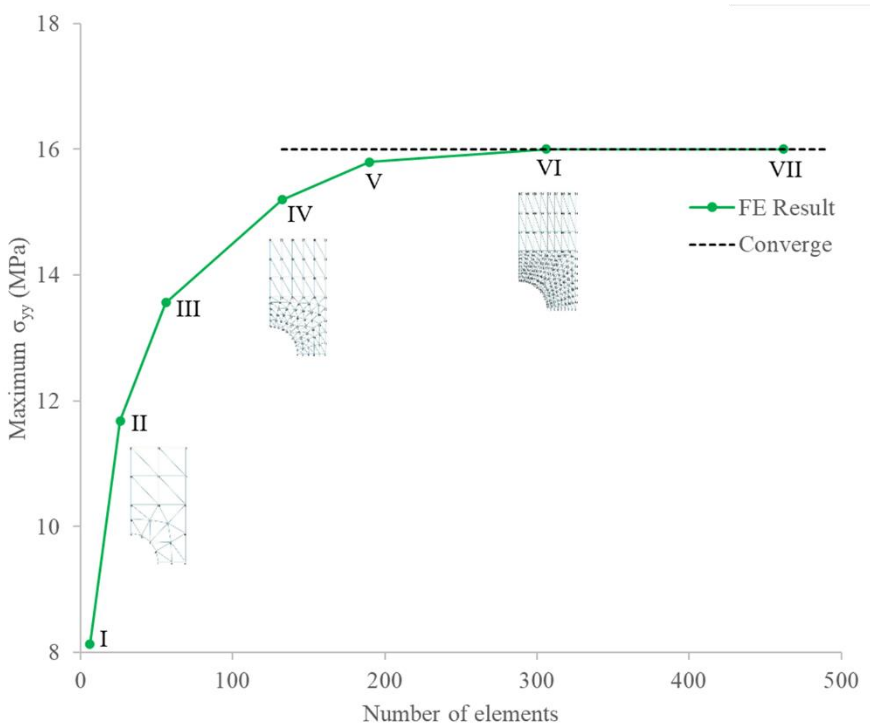


Figure 3 FEM plate model convergence study

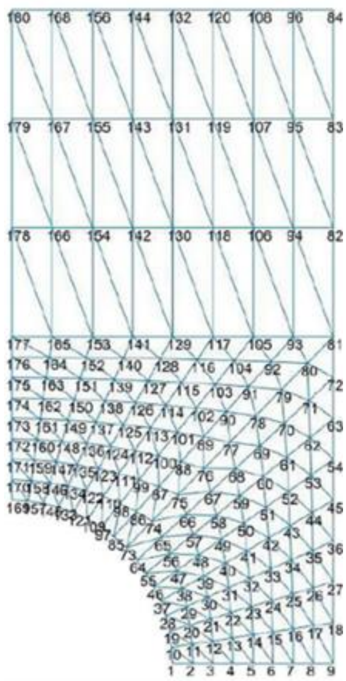


Figure 4 FEM model VI with 108 nodes and 304 elements

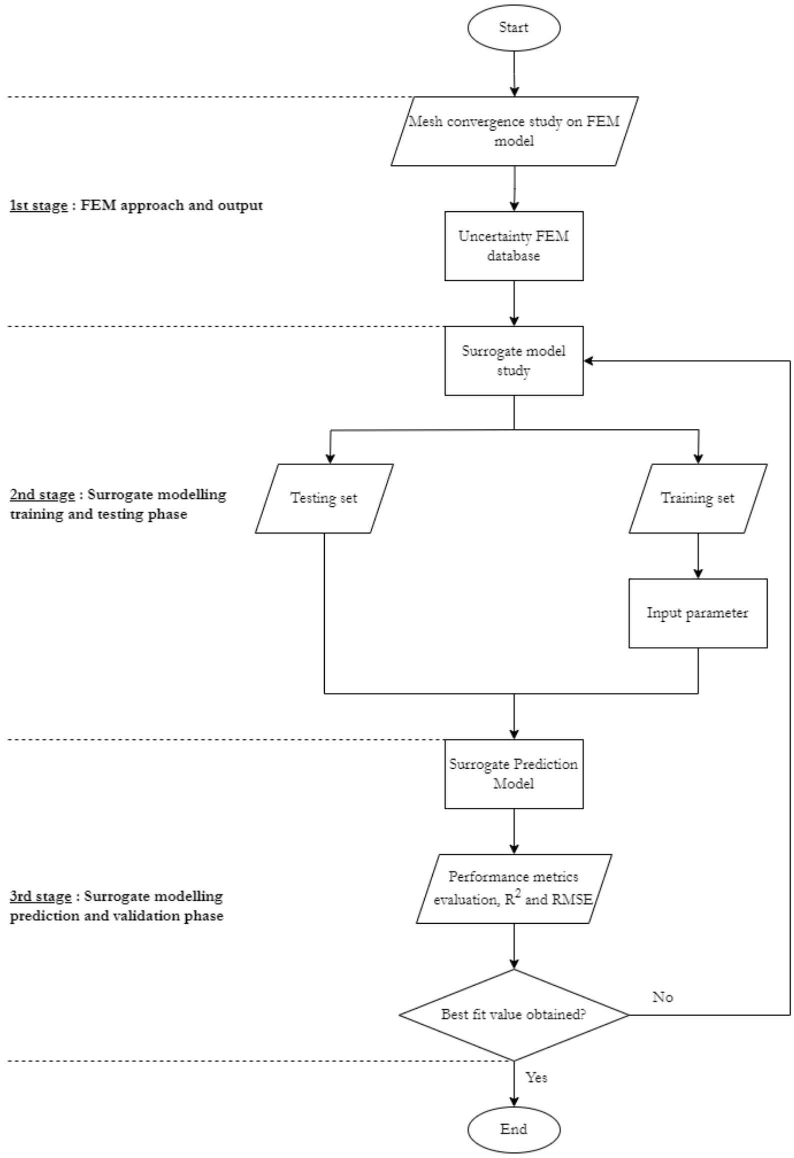


Figure 5 Flowchart of tasks

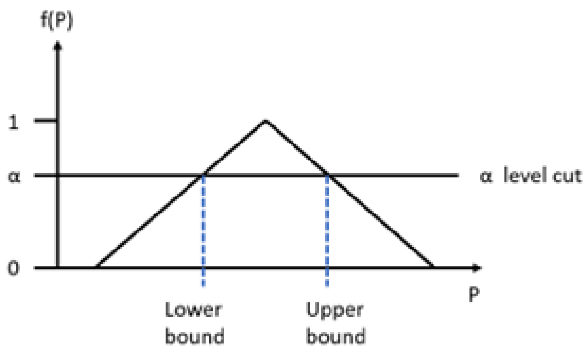


Figure 6 Fuzzy output

Table 1 Plate model specifications (Yanase, 2017)

Parameters	Value	Uncertainty Span
Young's modulus, *E*	222.5 GPa	±12.5 GPa
Distributed force, *F*	5500 N	±500 N
Poisson's ratio, *v*	0.32	±0.02

3.2 Uncertainty parameters

Stritih et al., (2019) highlighted those uncertainties existed due to information scarcity in process modelling. There are two types of uncertainties: aleatory and epistemic uncertainties. Aleatory is associated with the natural law, while epistemic uncertainty is related to the extent of human thinking. According to Faes, & Moens (2020), and Kamil et al., (2023), there are two uncertainty solution methods: the probabilistic and non-probabilistic approaches. This study applied the Monte Carlo simulation and fuzzy analysis approach, respectively. Combining the fuzzy analysis and Monte Carlo simulation creates the Fuzzy-Random approach. The parameters of the plate were set with a range of values, from minimum to maximum values, to perform FEM simulation on the plate with uncertainties.

The Monte Carlo simulation relies on recurrent arbitrary sampling and statistical analysis to perform computational simulation runs (Noii et al., 2022). This method requires a data set and randomly generates any numbers or data in the sample between a defined range of minimum and maximum limits. A loop system or function can be implemented to have a set of random data after each loop.

The fuzzy analysis technique is a non-probabilistic uncertainty method that involves fuzzy numbers mapping using α-cut based computational procedure and has fuzzy sets as the output (Baykasoğlu, & Gölcük, 2021; Das, & Granados, 2022; Zafwan et al., 2024). This procedure defines the output as lower and upper bound values representing the fuzzy sets. These fuzzy sets interpret numerical parameters into membership functions. Figure 6 depicts the lower and upper bounds of a fuzzy outcome of an element P. The triangle shape represents the membership function. The α-cut mapped f(P) output to a crisp set, the lower and upper bounds.

The uncertainty parameters in this paper are the plate's material properties, and the force applied. The uncertainty range was fixed in a span of maximum and minimum numbers. Table 1 represents the steel plate specifications: Young's Modulus, *E*; Poisson's Ratio, *v*; and distributed force, *F*. The uncertainty range of these specifications is presented in Table 1.

3.3 Surrogate Models

The number of uncertainty parameters can be increased to conduct a deep analysis of this study. However, this approach requires more computational effort, increased time consumption and increased cost. According to Alizadeh et al., (2020), the surrogate model technique is an alternative to this limitation. The surrogate model is an approximate simplified representation of a complex and computationally expensive system. It can be applied in machine learning techniques and for engineering predictions in simulations. The regular methods of surrogate models are DT and GPR. In this paper, both models were used for prediction.

3.3.1 Decision Tree (DT) method

Shivaie et al., (2021) proposed the decision tree method as a surrogate model approach. This white-box model has a visible and clear prediction mechanism. This method is a supervised machine learning technique replicating a model by prediction via classification and regression tasks (Kunviroteluck et al., 2024). This model is transparent, interpretable and resembles a tree system in making decisions based on an input's feature or parameters. It can handle both numerical and categorical parameters. In this tree system, a decision is reached based on a parameter at each internal tree node. Then, the parameter is split into branches representing the decision's outcome. Finally, the results or predictions are the leaf nodes of the branches. The features or parameters keep splitting into multiple subsets or decisions until each subset contains only one final decision. Figure 7 illustrates an example of a decision tree with its leaves and branches. V_1, V_2, and V_3 are the tree's features, P, Q, R, S, T, and U are the branches, and Decisions 1, 2, 3 and 4 are the leaves. In this study, the parameters in Table 1, Young's modulus, E, distributed force, F, and Poisson's ratio, v, are the tree's features and parameters. At the same time, the von-Mises stress (VM) and displacement are the leaves (decisions) produced by the tree.

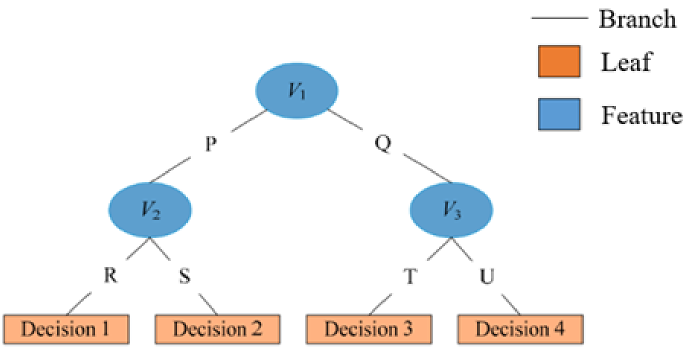


Figure 7 A decision tree with branches and leaves (Ahmad et al., 2020)

3.3.2 Gaussian Process Regression (GPR) method

Asante-Okyere et al., (2018) state that Gaussian Process Regression (GPR) is a surrogate model characterized by a straightforward function. This function describes the training data, incorporating uncertainty parameters from Table 1 and FEM outputs without the need for manual tuning of specifications. This model is a probabilistic non-parametric machine learning method for regression by defining a probability and function distribution to make predictions. It sets a preliminary allocation of vast possibilities over the function directly. This distribution includes a mean prediction and a measure of variance. The regression task helps to produce predictions that are continuous values, which are the von-Mises stress (VM) and displacement values. GPR relies on a covariance function, which is the kernel function. This function determines the shape and smoothness of an estimated function. It measures the similarity between the FEM data points. The kernel function has parameters learned from the input data in Table 1. These parameters influence the shape of a predicted function. Equation 1 shows the kernel function of a GPR.

Assume that a training set y of n number of parameters and an input matrix $x \in R^n$ and an output variable $y \in R$, the *GPR* equation is as follows;

$$y_* \sim GPR(m(x),k(x,x')) \qquad (1)$$

where *GPR* is the Gaussian Process Regression, *m(x)* is the mean function and *k(x,x')* is the covariance (kernel) function.

3.3.3 Training and prediction output process

A total of 100 sets of data were obtained from the Fuzzy-Random FEM simulation. This simulation was acquired by incorporating the uncertainty range of the input parameters into the Fuzzy-Random method in the FEM simulation. The output of this uncertainty simulation is an essential tool for a surrogate model's training and testing phase. This output data contains the input parameters and their corresponding results from the Fuzzy-Random simulation.

The totality of the data is separated for the training and testing phase. Fallucchi et al., (2020), and Esfe et al., (2021) suggested that the ideal portion of 70% of the data is for Training, while another 30% is for the testing phase. The training and testing phases are the main elements of surrogate modelling. The training data is used to construct the DT and the GPR model in the training phase. Once completed, the constructed model is evaluated to ensure it accurately represents the original model.

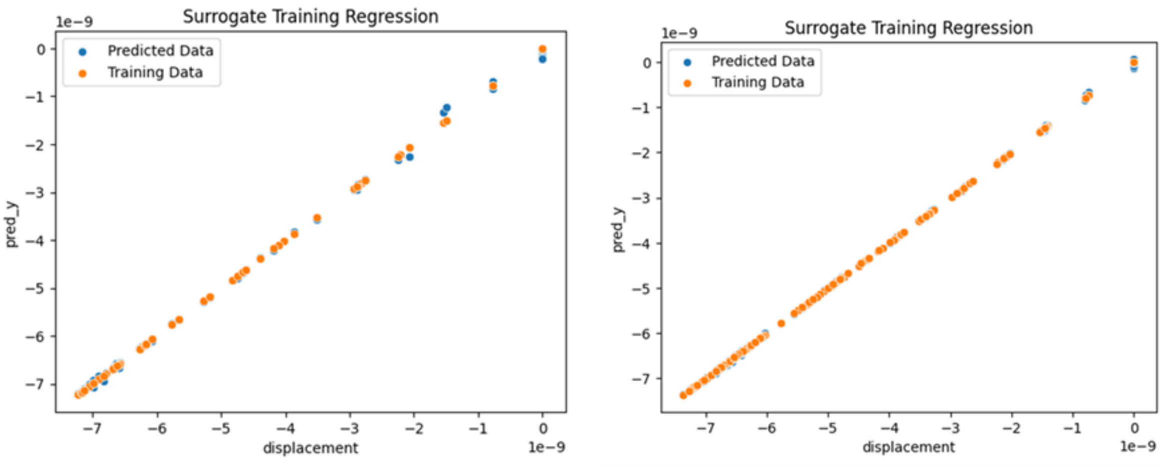
The testing phase assesses the model's performance and is used to compare the predicted output of the surrogate model with the original model. A performance metrics tool, the coefficient of determination, R^2, and the Root Mean Squared Error, RMSE, are used to measure the precision and validate the prediction output of the model. Figures 8 and 9 show the validation process of the surrogate model's prediction data with the original model's output. Figure 8 is the surrogate model's prediction output for the displacement of the plate. Figure 8(a) indicates the surrogate model prediction output has not yet achieved good regression with the original model's result with only 10 data, and its value of R^2 is 0.887 and RMSE is 0.436. Thus, the required training data quantity is insufficient to construct a perfect surrogate model of the original data. However, Figure 8(b) represents a good correlation of the surrogate model prediction with the original data, with a value of R^2 of 0.998 and RMSE of 0.012, with 30 training data.

Figure 9 is the surrogate model's prediction output for the stress von-Mises (VM) of the plate. Figure 9(a) shows the surrogate model prediction output has not yet achieved good regression with the original model's result with only 10 data, and its value of R^2 is 0.888 and RMSE is 0.512. However, Figure 9(b) represents a good correlation of the surrogate model prediction with the original data, with a value of R^2 of 0.999 and RMSE of 0.019, with 30 training data. Tang et al., (2020), and Asteris et al., (2021) have highlighted that a surrogate model can produce a precise and accurate prediction output when sufficient Training has been accomplished.

4. Results and Discussion

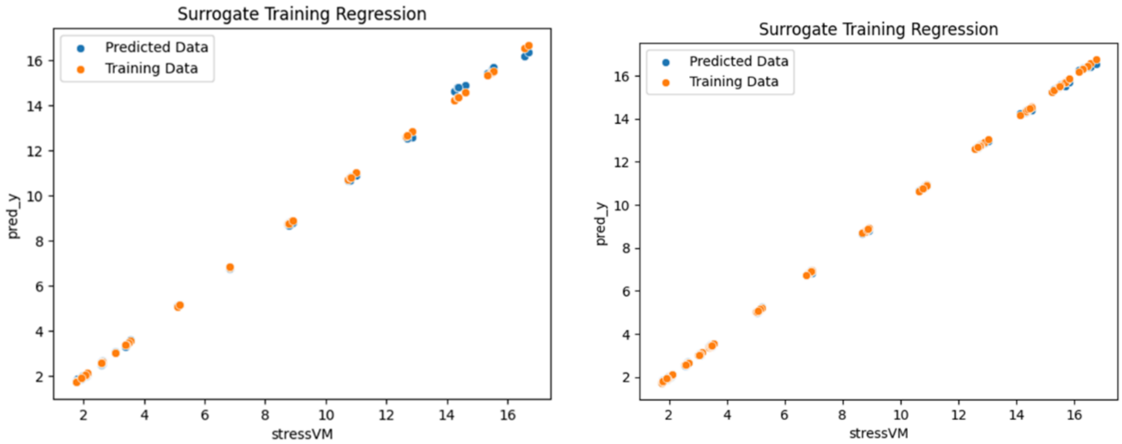
Two data sets were prepared as inputs for both surrogate models to produce prediction output. Each set consists of several values of data, which are the value of the force applied, *F*, Young's modulus, *E*, and Poisson's ratio, *v*. The first set of data consists of input parameters with deterministic or fixed values. In contrast, the second set consists of input parameters with random data values. This is to test the robustness of the surrogate models when there is a significant change in input parameters for prediction purposes. Figure 10 represents the comparison of the displacement output of the quarter plate via the FEM approach and the surrogate models, the GPR and DT methods. The prediction output of the surrogate models was compared to the FEM output, and the predictions were based on the first set of data. The FEM curve is the exact value and serves as the benchmark for the output of both models.

The three curves have a maximum displacement value at a 90° angle at the top edge of the plate's hole. The displacement was small but increased slowly with the angle. This shows that the force's vertical pull increased the plate's displacement. It is observed that both surrogate models' output curve has the same curve trend as the FEM output and are almost superposed with each other in the figure. The coefficient of determination, R^2, and the RMSE in Table 2 show that the value of R^2 and RMSE of both models was 0.998 and 0.017 for GPR and 0.997 and 0.022 for DT, respectively, when compared with the FEM output. Therefore, this shows a good validation of the surrogate model's output with the FEM result, as the R^2 value is close to 1 and the RMSE value is close to 0.



(a) 10 data (b) 30 data

Figure 8 Surrogate model validation output for displacement



(a) 10 data (b) 30 data

Figure 9 Surrogate model validation output for von-Mises stress

Table 2 Coefficient of determination, R^2 and RMSE for displacement

Surrogate Model	R^2	RMSE
GPR	0.998	0.017
DT	0.997	0.022

Table 3 Coefficient of determination, R^2 and RMSE for von-Mises stress

Surrogate Model	R^2	RMSE
GPR	0.998	0.015
DT	0.992	0.025

Figure 11 shows the comparison of the von-Mises stress (VM) output of the quarter plate via the FEM approach, the GPR and the DT methods. The prediction output of the surrogate models was compared to the FEM output, and the predictions were based on the first set of data. The FEM curve was the benchmark curve for comparison purposes.

The three curves have a maximum VM stress value at 0° angle at the lower edge of the plate's hole. The stress value was intense at 0° angle, decreased slowly from 60° to 70°, and then increased gradually after 70°. This shows that the vertical pull of the force exerted a high VM stress intensity at the fixed end of the plate (0°). It is observed that the output curves of both surrogate models follow the same trend as the FEM output and almost superposed with each other after 50° in the Figure 11. The R^2 and RMSE values in Table 3 for both surrogate models are 0.998 and 0.015 for GPR and 0.992 and 0.025 for DT, respectively, when compared with the FEM result. Therefore, this shows a good validation of the surrogate model's output with the FEM result, as the R^2 value is close to 1 and the RMSE value is close to 0.

Based on these results, both surrogate model methods can produce precise predictions using the first data set as input if 30 data sets were supplied to the surrogate models during the training phase. Therefore, it is essential to have adequate FEM data for the surrogate models' training purposes and for making prediction outputs (Tan et al., 2022; Jiang, & Durlofsky, 2023). Furthermore, these findings demonstrate that both surrogate models can simulate and produce prediction outputs by implementing input parameters with uncertainties and ranges.

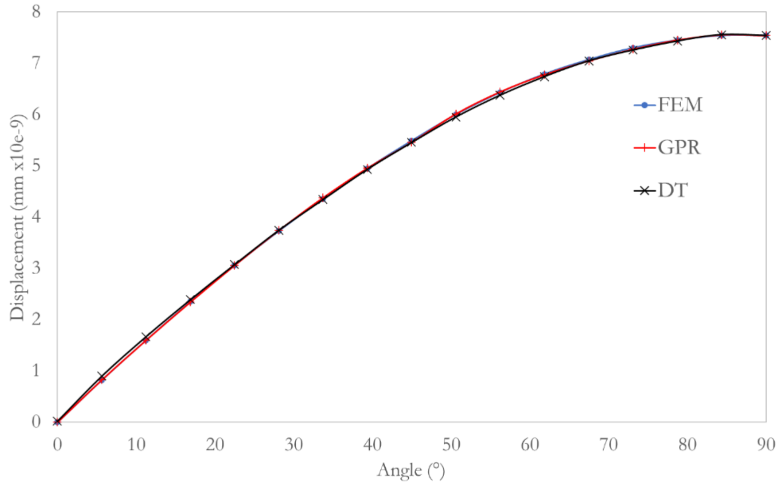


Figure 10 Displacement output of the quarter plate with deterministic input parameter

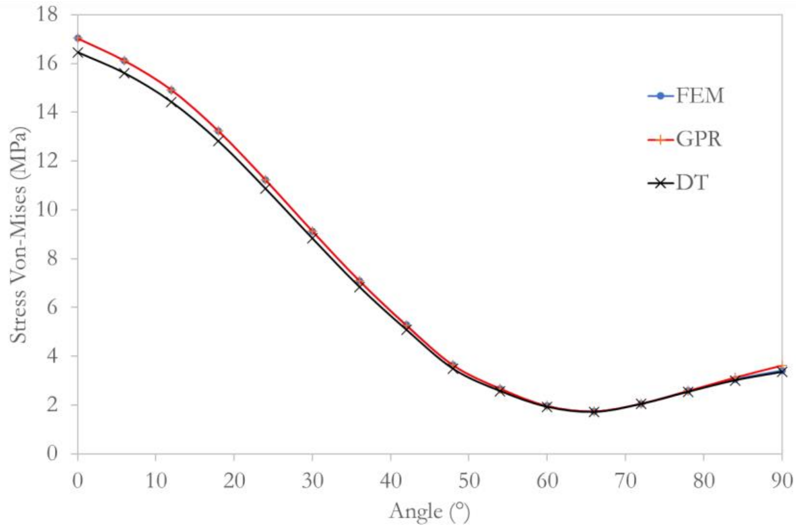


Figure 11 von-Mises stress output of the quarter plate with deterministic input parameter

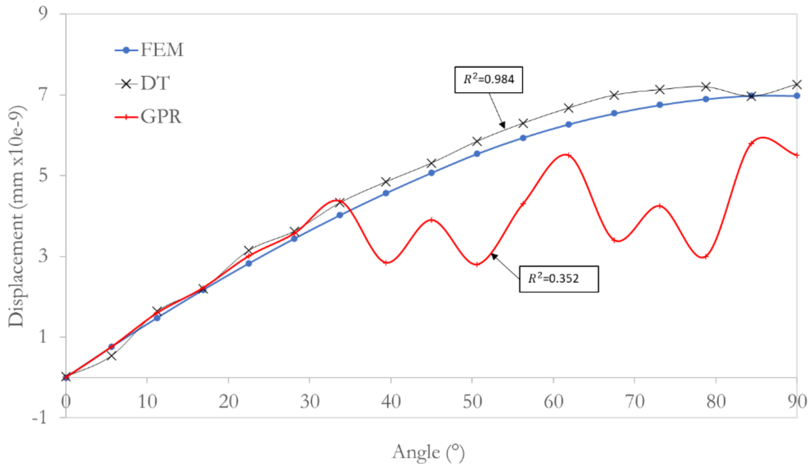


Figure 12 Displacement output of the quarter plate with random input parameter

Figure 12 illustrates the comparison of displacement output of the quarter plate via the FEM approach and the surrogate models, the GPR and DT methods. The prediction output of the surrogate models was compared to the FEM output, and the predictions were based on the second set of input data. The FEM curve was the benchmark curve for comparison purposes.

Similar to Figure 9, the FEM and DT curves have a maximum displacement value at a 90° angle at the top edge of the plate's hole. The displacement increased slowly with the angle. The DT output curve, with a coefficient of determination (R^2) value of 0.984 and an RMSE value of 0.031 when compared to the FEM output values. Therefore, this shows a good validation of the DT output with the FEM output. However, contrary to the DT model, the GPR model's curve failed to follow the same trend and trajectory as the FEM output curve. With a coefficient of determination (R^2) of 0.352 and an RMSE value of 0.674, this represents poor validation. The GPR curve only managed to follow the FEM curve trend before the 33° angle, and it failed to maintain the trajectory afterwards. Table 4 represents the value of R^2 and RMSE of both surrogate models.

Figure 13 compares the VM stress output of the quarter plate via the FEM approach, the GPR and the DT methods. The prediction output of the surrogate models was compared to the FEM output, and the predictions were based on the second set of input data. The FEM curve was the benchmark curve. The value of the VM stress was at its maximum point at 0° and had minimum values of 60° and 70°. The DT and VM output curves have the same curve trend and trajectory as the FEM output curve. The DT model's coefficient of determination, R^2, value is 0.999, and its RMSE value is 0.011, indicating good validation as the curves almost superpose on each other. However, the GPR model's output failed to follow the same curve trend and trajectory of the FEM curve. The GPR model's coefficient of determination, R^2, value is 0.471, and RMSE value is 0.531. They represent a poor validation value. Similar to Figure 10, the GPR curve only managed to follow the FEM curve trend between 6° and 36°, and it failed to maintain the trajectory afterwards. Table 5 shows the value of R^2 and RMSE of both surrogate models.

The simulation output results from Figures 11 and 12 demonstrate that the DT method is more robust than the GPR method. The DT method consistently maintain its prediction output performance, although there was a change in input parameters from deterministic to random data values. Chen et al., (2019), and Hafeez et al., (2021) highlighted that the DT approach is robust and can be applied in non-linear cases, proving that this surrogate model can be subjected to random input parameters for prediction purposes. Moreover, regression methods such as the GPR method only produce a scalar output value of Y, although a multi-variable input value of X is introduced. This limitation prevents the method from predicting consistent output values when a set of random values is used as input parameters (Kaneko, 2021).

Table 4 Coefficient of determination, R^2 and RMSE for displacement

Surrogate Model	R^2	RMSE
GPR	0.352	0.674
DT	0.984	0.031

Table 5 Coefficient of determination, R^2 and RMSE for von-Mises stress

Surrogate Model	R^2	RMSE
GPR	0.471	0.531
DT	0.999	0.011

Table 6 Simulation time (s) for uncertainty FEM and surrogate model

Total data	10	30	50	70	100
Uncertainty FEM	300s	840s	1380s	1890s	2700s
Surrogate model (DT)	4.37s	5.58s	8.7s	21s	40s

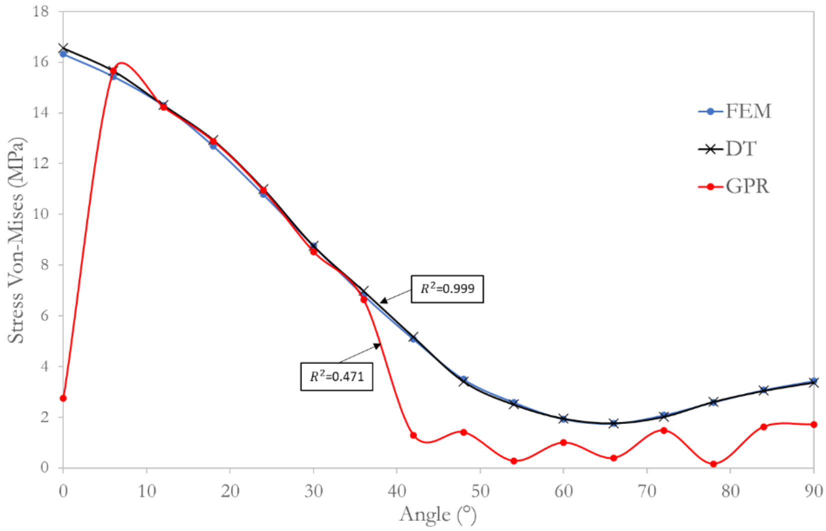


Figure 13 von-Mises stress output of the quarter plate with random input parameter

Table 6 shows the comparison of the simulation running time of the surrogate model, the DT method, and the uncertainty FEM with the total input data used in the simulation for output prediction purposes. The simulation was performed for 100 input data, and the time was in seconds. Only the DT method time simulation is considered, showing promising results and predictions for both inputs. Based on Table 6, the number of data sets applied to the surrogate model to produce output prediction did not significantly impact the time to complete a simulation run. The simulation time curve was almost constant until 100 data in total. However, the uncertainty FEM simulation time curve has significantly increased from 0 to 100 data sets. The simulation time for the surrogate models was observed to be more than three times faster than the uncertainty FEM output, and it shows that the total amount of data in the surrogate models has no evident impact on the simulation run time. As for the uncertainty FEM approach, a more significant increase in the number of input data increases the complexity of the FEM model (Luo et al., 2022), and this requires more computational effort and simulation time. Huzni et al., (2022) mentioned that a complete simulation time run of a surrogate model is four times faster than a full computing time of a FEM approach. The surrogate model approach represents a "trade-off" between computational effort, cost, and simulation time.

5. Conclusion

This research focuses on the capability of surrogate models, the DT and GPR methods, to produce predictions with uncertain input parameters. A finite element model is created, and the material specifications and boundary conditions are the uncertainty properties. Uncertainty FEM was performed with the implementations of the Fuzzy-Random approach. The simulation output was then compared to the output of the surrogate models, and two performance metrics tools, the coefficient of determination, R^2 and the Root Mean Squared Error, RMSE, were used to measure the accuracy of the prediction.

Both surrogate models have excellent and accurate prediction output when applying a deterministic input parameter for prediction purposes. However, when a random input parameter was used, the DT method outperformed and was more robust than the GPR method. The DT method still maintains accurate prediction with an R^2 value of 0.999 and an RMSE value of 0.011.

Moreover, simulations using surrogate models are three times faster than those using the FEM method to produce output. This demonstrates that the surrogate model can be an alternative method for computational and cost efficiency, high fidelity and precision, and simulation time reduction when compared to the FEM method. However, this approach depends on input data for training and prediction, such as output data from FEM simulations, and cannot function independently. Future research can compare the neural network approach, Bayesian Network and Artificial Neural Network (ANN) with the DT method regarding prediction output performance.

6. Acknowledgements

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