PERFORMANCE EVALUATION OF MACHINE LEARNING ALGORITHMS FOR REGRESSION OF FINITE ELEMENT ANALYSIS (FEA) SIMULATION DESIGN DATA

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Abstract: The process of developing the design for new parts and structures through FE simulations demands significant human and computational effort. By employing the multi-objective optimization method using DOE and metamodels, it is possible to achieve optimal design parameters faster and with greater precision. Thus, this study assessed the efficiency of using Machine Learning as metamodels to represent the behavior of FE models. Conventional methods were trained with and without data normalization and standardization, employing cross-validation and hyperparameter tuning. Ultimately, this analysis provides the best models for different types of design data, making their utilization viable in certain cases.

Keywords: machine learning; multi-objective optimization; finite element analysis.

AVALIAÇÃO DO DESEMPENHO DE ALGORITMOS DE MACHINE LEARNING PARA REGRESSÃO DOS DADOS DE DESIGN DE SIMULAÇÃO DE ANÁLISE DE ELEMENTOS FINITOS (FEA)

Resumo: O processo de desenvolvimento do design de novas peças e/ou estruturas através de simulações FE requer muito esforço humano e computacional. A utilização do método de otimização multi-objetivo através do uso do DOE e de metamodelos é possível obter resultados de parâmetros de design ótimos mais rápido e com maior precisão. Assim, este trabalho avaliou a eficiência da utilização de Machine Learning como metamodelos para representar o comportamento dos modelos FE. Os treinamentos dos métodos convencionais, sem e com normalização e padronização dos dados, foram feitos utilizando validação cruzada e o ajuste dos hyperparâmetros. Finalmente, está análise fornece os melhores modelos para diferentes tipos de dados de design, sendo viável a sua utilização em alguns casos.

Palavras-chave: aprendizado de máquina; otimização multi-objetivo; análise de elementos finitos.

1. INTRODUCTION

The process of developing new parts and/or structures in engineering has undergone significant advancements due to the increase in computational power. However, in some cases, there are still challenges related to the high complexity of the relationship between parameters and performance metrics. Typically, the development process involves successive iterations of design creation, simulation, and analysis, requiring significant efforts from the engineer and computational resources until optimal metrics are achieved with parameters within the constraints [1]. As a result, some methods have emerged to expedite and facilitate this process, among which Finite Element Analysis (FEA) combined with an optimization algorithm stands out for its higher accuracy [2,3].

However, when dealing with the design modeling of new parts using FEA, there is a relationship between numerous parameters and objectives, making it a multi-objective optimization problem. In such cases, the goal is to simultaneously minimize or maximize the values of the objective equations by altering the parameters to find the set of optimal solutions, known as the Pareto Front [4]. There are two ways to optimize the design variables: by combining the optimization algorithm with a direct design method or with metamodels resulting from the Design of Experiments (DOE). Metamodels are mathematical models capable of approximating the relationships between variables and responses. As for DOE, it is a statistical application used to design experiments and analyze the results to identify relationships between design variables and responses. Through multi-objective optimization by creating metamodels from DOE, it is possible to obtain optimal results while analyzing the sensitivity between parameters and responses of the Finite Element (FE) model [3,5].

Recently, there have been many studies on multi-objective optimization using metamodels. Traditional statistical models such as linear regression, logistic regression, and polynomial regression can be used as metamodels, yielding good results for simpler systems. However, they have shown limitations in handling more complex systems with large amounts of data, parameters, and nonlinear relationships. In this context, Machine Learning (ML) comes into play to overcome these limitations, as it demonstrates better performance due to its adaptability features [3,6]. Therefore, this study aims to evaluate the performance of conventional ML techniques as metamodels for design variables with more than one objective response.

2. METHODOLOGY

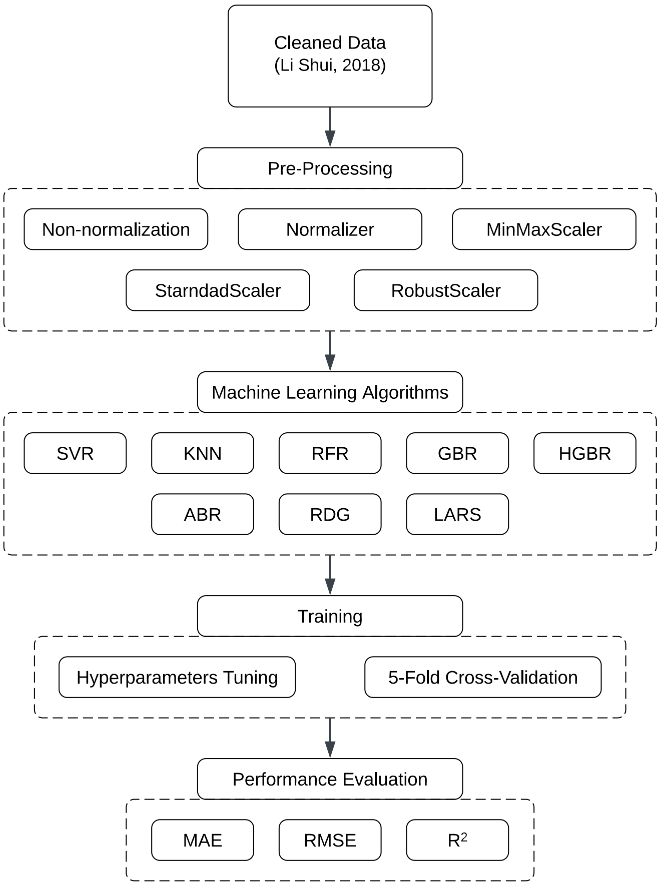
For this study, the machine learning algorithms were modeled, and their accuracy was statistically evaluated. The methodology was divided into four main steps: data acquisition and pre-processing, algorithm modeling and normalization, model training and hyperparameter tuning, and statistical analysis of model performance.

The data used in this study was extracted from the work of Shui et al. 2018, which involves multi-objective optimization of design parameters for an electric vehicle battery enclosure. The ANSYS software was utilized for basic design modeling and finite element analysis to obtain the design data and responses to variations in the dimensions of the component. Design of Experiments (DoE) was employed, specifically the Central Composite Design (CCD) method, to define 100 different simulation samples, varying the design parameters (battery box thickness (EW), bottom box thickness (EB), module bottom thickness (bb), battery module long wall thickness (bwl), battery module wide wall thickness (bww), and ambient temperature) and determining the maximum deformation (maxdef), minimum natural frequency (minfreq), and mass (mass) [7].

For the prediction of the aforementioned metrics, conventional regression machine learning algorithms were employed. These included Support Vector Regression (SVR), K-Nearest Neighbors Regressor (KNN), Random Forest Regressor (RFR), Gradient Boosting Regressor (GBR), Histogram Gradient Boosting Regression (HGBR), AdaBoost Regressor (ABR), Ridge Regressor (RDG), and Least Angle Regression (LARS). In addition to using these regression algorithms, various data normalization and standardization methods applicable to numerical data were applied. These methods include Normalizer, MinMaxScaler, StandardScaler, and RobustScaler, along with evaluating the algorithms without any normalization. These techniques are used to ensure that the input data is within a specific range or distribution, which can aid in improving the performance of the machine learning models and their predictions.

The database was divided into 75% for training and 25% for testing. With the training set, a 5-fold cross-validation was applied to enhance the robustness and effectiveness of the models. Hyperparameter tuning was performed for all models to optimize their performance. After the training and identification of the best estimators, model evaluation was conducted using the remaining 25% of the database. The evaluation metrics used to assess the accuracy were the Mean Absolute Error (MAE), Root Mean Squared Error (RMSE), and the Coefficient of Determination (R2). Figure 1 illustrates the structure of the proposed method, depicting the entire workflow of data division, model training, cross-validation, hyperparameter tuning, and final model evaluation.

Figure 1. Flowchart of the proposed methodology



3. RESULTS AND DISCUSSION

With the training and hyperparameter tuning completed, the R2 of the best models obtained for each analyzed output was calculated. The results for maximum deformation (maxdef), minimum natural frequency (minfreq), and mass (mass) are presented in Tables 1, 2, and 3, respectively.

Table 1. Best scores "maxdef"

	SVR	KNN	RFR	GBR	HGBR	ABR	RDG	LARS
Sem normalização	-0.354564	-0.298877	0.441002	0.491543	0.387485	0.32401	0.41419	0.413747
Normalizer	-0.354564	-0.17981	-0.275857	-0.255419	-0.219197	-0.16473	-0.213412	-0.199506
MinMaxScaler	-0.354564	0.304519	0.44542	0.492874	0.384867	0.314216	0.420129	0.413747
StandardScaler	-0.354564	0.3057	0.457914	0.484489	0.383447	0.273299	0.420626	0.413747
RobustScaler	-0.354564	0.288695	0.46121	0.498929	0.387485	0.295005	0.417436	0.413747

In maximum deformation, it is observed that none of the models performed adequately, likely due to the models' incapacity to handle the relationship between the design parameters of the component and deformation. The work of Li Shui demonstrated an 85% contribution of the parameters to this objective. Notably, the SVR model performed poorly, as seen in Figure 2 below, for the SVR model without normalization. The low MAE and RMSE values are correlated with the extremely low variation between the maximum and minimum values. Meanwhile, the GBR model achieved the best results, but still with an unacceptable performance.

Figure 2. Prediction of "maxdef" with the SVR model without normalization

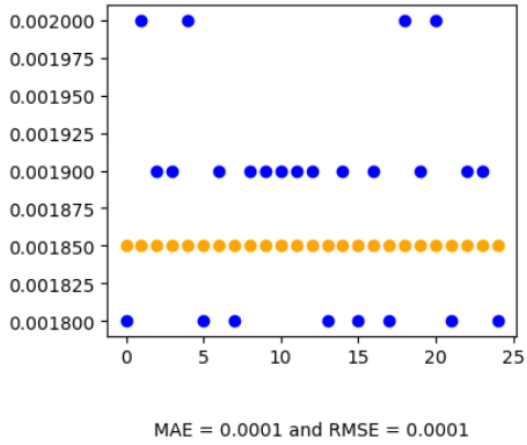
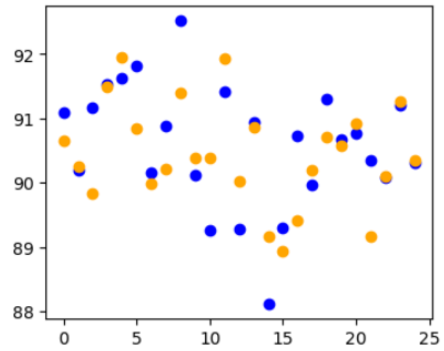


Table 2. Best scores “minfreq”

	SVR	KNN	RFR	GBR	HGBR	ABR	RDG	LARS
Sem normalização	0.710415	-0.014857	0.558762	0.605467	0.381865	0.516432	0.70262	0.69846
Normalizer	0.220715	0.098472	0.241048	0.22525	0.308989	0.265679	0.02328	0.506411
MinMaxScaler	0.716896	0.489414	0.572477	0.615199	0.380361	0.549838	0.701917	0.69846
StandardScaler	0.726607	0.444065	0.565039	0.600944	0.381865	0.547135	0.7002	0.69846
RobustScaler	0.716382	0.432812	0.556956	0.602005	0.381865	0.564704	0.699917	0.69846

In the minimum natural frequency models, a significant improvement in the best scores is evident, with the SVR, RDG, and LARS models standing out positively. These models demonstrate the capability to generalize with small deviations from the actual values, as shown in Figure 3.

Figure 3. Prediction of "minfreq" with the SVR model without normalization



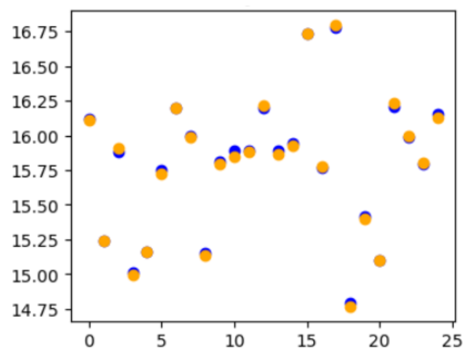
MAE = 0.5182 and RMSE = 0.6842

Table 3. Best scores "mass"

	SVR	KNN	RFR	GBR	HGBR	ABR	RDG	LARS
Sem normalização	0.999666	0.006834	0.719777	0.815092	0.71168	0.732646	0.999582	0.955331
Normalizer	-0.007921	-0.057203	-0.107559	-0.015437	-0.049007	-0.078389	-0.028437	-0.237806
MinMaxScaler	0.999641	0.76399	0.721462	0.815588	0.711897	0.725814	0.999628	0.999642
StandardScaler	0.999648	0.767573	0.725271	0.810552	0.712153	0.728443	0.999643	0.999642
RobustScaler	0.999641	0.76867	0.720033	0.816804	0.712153	0.738887	0.999643	0.999642

The best objective for which the models showed the best fit was the mass, as seen in Figure 4, with R2 values above 0.71. The models' better adaptation to the mass is related to its direct and linear relationship with the dimensions of the component. Since mass is directly influenced by the dimensions of the design parameters, the models were able to capture this relationship effectively, resulting in higher R2 values and better predictive performance for the mass objective.

Figure 4. Prediction of "mass" with the SVR model without normalization



MAE = 0.0153 and RMSE = 0.0181

In addition to the presented results, there are two important observations to be made. First, the Normalizer method showed poor results in all analyzed objectives and models, as it normalizes each sample individually, which may not be suitable for the data distribution and relationships within the dataset. Second, the K-Nearest Neighbors (KNN) method without normalization also had poor results without any plausible justification.

4. CONCLUSION

The study aimed to analyze conventional machine learning (ML) methods with various data normalization and standardization techniques, in addition to hyperparameter tuning. For this purpose, exploratory training was performed using preprocessed data, followed by testing with previously unused data to evaluate the effectiveness of the suggested models. The results obtained were satisfactory for the given dataset. It is recommended to use the Support Vector Regression (SVR) model without normalization for the objectives "minfreq" and "mass" due to its high accuracy and fast training and prediction capabilities. Additionally, the Gradient Boosting Regressor (GBR) model is suggested with any normalization technique, except for the Normalizer method, for the "mass" objective.

5. REFERENCES

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