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MACHINE LEARNING-BASED PREDICTION OF WÖHLER CURVES FOR Ck35 STEEL

PRIMENA MAŠINSKOG UČENJA U PREDVIĐANJU VELEROVIH KRIVIH ČELIKA Ck35

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Keywords
- S-N curve
- machine learning
- Support Vector Machine
- Gaussian Process Regression

Abstract

Machine learning has become a powerful tool for prediction and discovery by learning patterns from observations, although its reliability depends on appropriate model selection, rigorous evaluation, and awareness of inherent limitations. This study investigates the prediction of S-N behaviour of Ck35 steel (DIN EN 10083) using three machine learning models: Support Vector Machine (SVM), Linear Regression (LR), and Gaussian Process Regression (GPR), implemented in MATLAB®. A material identifier extracted from sample codes is used to partition the experimental dataset into distinct groups, with available fatigue data in each group alternately divided into training and test sets. To capture the expected S-N relationship, both stress amplitude and number of cycles to failure are transformed to a logarithmic space. Each model is trained separately to predict fatigue life as a function of applied stress, and performance is evaluated using Mean Absolute Percentage Error and Root Mean Square Error metrics. The SVM and GPR models demonstrate better predictive performance compared to classical LR, particularly for nonlinear data groups. Each predicted group and experimental S-N curve are compared to assess accuracy, illustrating the potential of machine learning approaches to reduce the scope of experimental fatigue testing through the application of intelligent algorithms.

Ključne reči
- S-N kriva
- mašinsko učenje
- Metode potpornih vektora
- Regresije Gausovim procesima

Izvod

Mašinsko učenje je postalo moćan alat za predviđanje i otkrivanje zakonitosti putem učenja obrazaca iz opservacija, mada njegova pouzdanost zavisi od adekvatnog izbora modela, rigorozne evaluacije i svesti o inherentnim ograničenjima. Ova studija analizira primenu tri modela mašinskog učenja: Metode potpornih vektora (eng. SVM), linearne regresije (eng. LR) i regresije Gausovim procesima (eng. GPR), sa ciljem predviđanja zamornih osobina (tačnije, S-N zavisnosti) čelika Ck35 (prema DIN EN 10083) u logaritamskom prostoru sadržanom u alatu MATLAB®. Eksperimentalni podaci su, nakon particionisanja pomoću identifikatora materijala, podeljeni na skupove za trening modela i testiranje istih sa ciljem predviđanja veka zamora u funkciji primenjenog napona. Evaluacija performansi ispitanih modela, sprovedena primenom metoda Srednje apsolutne procentualne greške i Korena srednje kvadratne greške, ukazuje na to da SVM i GPR modeli pružaju veću preciznost u odnosu na klasičnu linearnu regresiju, naročito kod nelinearnih skupova podataka. Uporedna analiza predviđenih i eksperimentalnih zamornih krivih potvrđuje tačnost predloženog pristupa, čime se ilustruje značajan potencijal inteligentnih algoritama u optimizaciji i smanjenju obima eksperimentalnih ispitivanja zamora materijala.

INTRODUCTION

Fatigue behaviour of materials is commonly described using Wöhler (S-N) curves, which relate stress amplitude (S) to the number of cycles to failure (N). Fatigue is one of the most critical failure mechanisms in metallic materials subjected to long-term cyclic loading, and it is especially dangerous because it occurs without prior warning. Modelling S-N curves based on results obtained by experimental testing is usually used to predict the service life of components in aerospace- /1, 2/, automotive industry /3, 4/, civil infrastructure /5-8/, railway infrastructure /9, 10/ and energy facilities /11-12/. A wide range of fatigue failure cases is documented in the ASM Handbook: Failure Analysis and Prevention /13/, and S-N curves are provided in the Atlas of Fatigue Curves /14/.

Although the classical fracture mechanics approach has been employed as a reliable tool for a long time up to the present /15-21/, data-driven models have emerged as substitutes for experimental fatigue testing, requiring adequate and optimal experimental datasets. Figure 1 illustrates the new machine-learning programming (more precisely, training) paradigm that replaces the traditional approach where rules and data are inputs processed by classical programming to yield answers. Machine learning inverts traditional approach by analysing input data in conjunction with their corresponding outcomes to infer the governing rules /22/. In other words, by analysing observations, a machine learning model

derives internal patterns (rules in Fig. 1) that it then uses to make predictions. As a result, machine learning has become central to prediction, explanation, and discovery across many fields - but its success depends on choosing appropriate models, evaluating them rigorously, and recognizing their limitations.

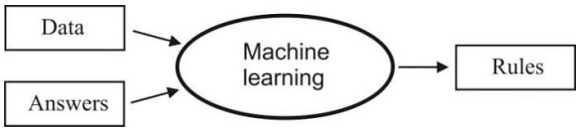

Figure 1. Illustration of the machine learning concept as a new programming paradigm, /22/.

Support Vector Machines (SVM), Linear Regression (LR), and Gaussian Process Regression (GPR) are established machine learning techniques used to generate data-driven estimates using supervised training. By modelling complex input-output relationships, these methods can be trained on experimental subsets to predict fatigue life under untested conditions which reduce the need for physical testing. Nowadays, machine learning methods are used for a wide range of purposes. For example, in the field of materials science, Lian et al. /23/ apply the gradient boost regression method to predict the fatigue life of seven different aluminium alloys. The S-N curve can be accurately estimated by combining the prediction of fatigue limit and the number of cycles to failure at a given stress amplitude, as in /24/. A novel method to predict the S-N curve is proposed by Wei et al. /25/, combining the Long Short-Term Memory (LSTM) network and transfer learning. A method for predicting the S-N curve of composite materials is proposed based on TR-LSTM neural network model of wind turbine blades in /26/. Arvanitis et al. /27/ proposed four methods that effectively leverage material preprocessing details, mechanical properties, and experimental conditions to accurately predict the remaining fatigue lifespan of structural steels using Polynomial Regression, Support Vector Regression, eXtreme Gradient Boosting Regression, and Artificial Neural Network. The application of different data science techniques, including feature selection and predictive modelling, to the analysis of fatigue properties of steels is discussed by Agrawal et al. /28/. From a fracture mechanics perspective, Ivković et al. /29/ demonstrated the feasibility of using Neural Network approach to determine fracture toughness and fatigue limit values for several grades of stainless steel.

In this study, a comparative machine learning framework comprising aforementioned SVM, LR, GPR is implemented to estimate fatigue stress amplitudes in S-N curves. These models are trained and validated using experimental fatigue datasets /30/ for three distinct grades of Ck35 steel, conducted within the scope of the FABER project. The experimental dataset is initially log-transformed to linearise the inherently exponential relationship between stress amplitude (S) and remaining fatigue life (N), enabling more effective computational modelling. The models are trained on alternating pairs of data subsets and validated using Mean Absolute Percentage Error (MAPE) and Root Mean Square Error (RMSE) metrics /31/. This evaluation aims to compare performance and accuracy of the three modelling methods, assessing their potential for predicting fatigue life in engineering applications. The data are derived from the 'BaB' test group of the previously mentioned open-source experimental dataset, /30/.

MATERIAL AND METHODS

Ck35 is German designation for quenched and tempered medium-carbon steel, commonly used in mechanical engineering applications for machine components such as shafts, gears, axles, flanges, forgings, connecting rods, and other structural parts. Carbon share is approximately 0.32-0.39 %, and contains small amounts of other elements such as silicon, manganese, sulphur, chromium, molybdenum and nickel.

In this study, the specimens for fatigue testing are fabricated from a tube /30/. Figure 2 shows the characteristic geometry of specimens, while Table 1 lists their dimensions, which are relevant for potential S-N predictions. Table 2 shows the basic mechanical properties of Ck35 steel.

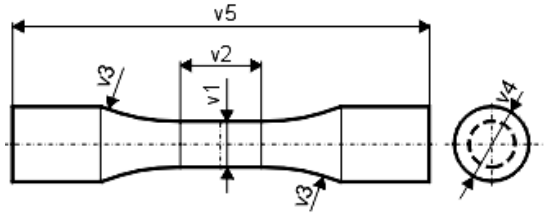

Figure 2. Technical drawing of the specimen, /30/.

Table 1. Numerical values of specimen dimensions.

Dimensions / specimen designation	BaB 010	BaB 020	BaB 030	BaB 040	BaB 060	BaB 070	BaB 080
v1- diameter [mm]	21	21	21	21	21	21	20
v2 - active length [mm]	15	15	15	15	15	15	0
v3 - fillet radius [mm]	40	40	40	40	40	40	40
v4 - diameter of fixture [mm]	26	26	26	26	26	26	26
v5 - total length [mm]	98	98	172	172	172	172	98

Table 2. Mechanical properties of steel Ck35.

Tensile yield stress [MPa]	Ultimate tensile strength [MPa]	Shear yield stress [MPa]	Hardness (Vickers) [-]
313	550	169	~ 148

To predict the S-N curves from the experimental dataset, the three previously mentioned machine learning models are applied:

1. Support Vector Machine (SVM)
2. Linear Regression (LR)
3. Gaussian Process Regression (GPR)

All three models are implemented and tested in MATLAB 2024b software package. The utilised experimental data consisted of S and N values for several specimen groups, labelled with suffixes ranging from 010 to 080 (see Table 1). Each sample is assigned to its respective group based on its identifier, and the corresponding S and N values are recorded. This grouping is necessary to enable a more efficient learning process and to match the data with the S-N curve '*nature*' (typically shown in log-log units). The input parameters for the models are log10(*N*) and log10(*S*). The dataset is divided into training and test sets using a fixed sampling scheme: those labelled {1, 3, 5, …} are used for training, while those labelled {2, 4, 6, …} are reserved for testing (validation). Note that this approach is adopted to minimize subjective bias in the model evaluation.

The following section outlines the theoretical foundations of 3 machine learning methods employed here. Finally, all models are evaluated using MAPE and RMSE metrics.

Support Vector Machine

The SVM model is used for regression, with the Radial Basis Function (RBF) as the kernel function. The RBF kernel allows the model to handle the nonlinearity between cycle number and stress. During training, core and regulation parameters are automatically adjusted. Prediction is performed on test data in logarithmic space, after which the results are returned to linear space by exponentiation. The *fitrsvm* function from MATLAB is used for implementation, with RBF as the core of the model. The nonlinear kernel function allows the model to perceive complex relationships between inputs and outputs, which are especially important for nonlinear dependencies such as S-N curves in some cases. The RBF kernel model has the following mathematical form:

$$K(x,X)=\exp\left(-\gamma\|x-x'\|^2\right),\quad \gamma=\frac{1}{2l^2}, \tag{1}$$

where: x is input vector of a training sample (in this case, log10(N)); x' is a test point where a prediction is desired; $\|x-x'\|^2$ is squared Euclidean distance between two points for multidimensional inputs (where $\|\ \|$ denotes Eucledean norm); γ is the kernel parameter controlling the width of the kernel, related to the length scale l (determining how quickly correlations decay and thus the flexibility of the model) /32/. The kernel function, represented by Eq.(1), evaluates similarity between x and x'.

The SVM model is here applied in the following steps:

1. For each group of samples, $\log_{10}(N)$ as input vectors and $\log_{10}(S)$ as target values are selected.
2. The training set is formed based on every other point {1, 3, 5, …} while the remaining points are left for model testing.
3. The *fitrsvm* model is trained with default parameters and the RBF kernel. The software itself automatically adjusts the hyperparameter.
4. After training, the model is used to predict $\log_{10}(S)$ values on the test set, which are then transformed back to linear space using exponential law.
5. Based on comparison with actual stress values, MAPE is calculated as one of the key accuracy metrics.

Linear regression

A standard LR is performed using the *polyfit* function in MATLAB 2024b, fitting an affine function of the form given in Eq.(2) in logarithmic space:

$$\log_{10}(S)=a\log_{10}(N)+b\log_{10}(S)=a\log_{10}(N)+b. \tag{2}$$

As the model assumes an affine relationship between log-transformed values, the data are transformed as follows:

$$x=\log_{10}(N),\quad y=\log_{10}(S), \tag{3}$$

to enable the application of the LR model to the typically exponential relationship between stress and the number of cycles characteristic of S-N curves. This transformation converts the exponential relationship into an affine one, enabling the use of an affine model expressed as:

$$y=ax+b, \tag{4}$$

where: x and y are as defined in Eq.(3); a represents the slope; and b denotes the offset (intercept).

The *polyfit* function, used to implement the LR model in MATLAB, determines the coefficients of the affine model by minimizing the least squares error (the best data fit in the least squares sense).

Gaussian Process Regression

GPR is a nonlinear model that provides predictions along with an associated uncertainty estimate. In this study, it is employed to model the relationship between the stress amplitude and the number of cycles to failure in S-N curves, using the data transformed into log-log space as in Eq.(3) for the previous model.

Mathematically, the GPR model assumes that the training data, together with the (testing) points we wish to predict, are jointly distributed according to a multivariate normal distribution defined by the kernel function. Therefore, the key GPR mean prediction formula is given by, /33/:

$$\hat{y}_*=k(x_*,X)^T\cdot[K(X,X)+\sigma_n^2\delta_{kk}]^{-1}\cdot y, \tag{5}$$

where: $\hat{y}_*$ is predicted mean at the test input (point) x_*; x_* is test point; X are training input data (points), $\log_{10}(N)$; $k(x_*, X)^T$ is the covariance vector between test point x_* and all training points X; $K(X, X)$ is covariance matrix of training inputs; y is the vector of training target values, $\log_{10}(S)$; $\sigma_n^2 I$ is noise variance (observation noise) to the covariance matrix diagonal (models uncertainty in the training outputs).

In the kernel function, this study uses the Squared Exponential Kernel (a default in MATLAB) which has the following form:

$$k(x,x')=\sigma_f^2\exp\left(-\frac{(x-x')^2}{2l^2}\right), \tag{6}$$

where: σ_f^2 is the parameter that controls amplitude (vertical variations) of the function outputs; l is length scale previously defined in conjunction with Eq.(1); and $(x-x')^2$ is the squared Euclidean distance between two points which generalises to $\|x-x'\|^2$ for multidimensional inputs, as given in Eq.(1), /33/. Notably, the Squared Exponential (SE) kernel used in GPR, represented by Eq.(6), and the RBF kernel commonly used in SVM, Eq.(1), are essentially the same type of kernel, just named differently in different contexts. Both kernels measure similarity (covariance) based on the distance between points, with similarity decreasing exponentially as points move farther apart.

TRAINING AND RESULTS

The data are grouped according to the first 6 characters of each specimen label. In some cases, groups defined in this way contain fewer than 6 valid data points; only groups with at least 6 valid points are included for model development. For each group, 3 independent models are trained:

- SVM with the RBF kernel function,
- LR with the least-squares fit, and
- GPR as approach that quantifies uncertainty in estimates.

Figure 3 shows a visual comparison of the estimates produced by all three models alongside actual curves, training data, and test data.

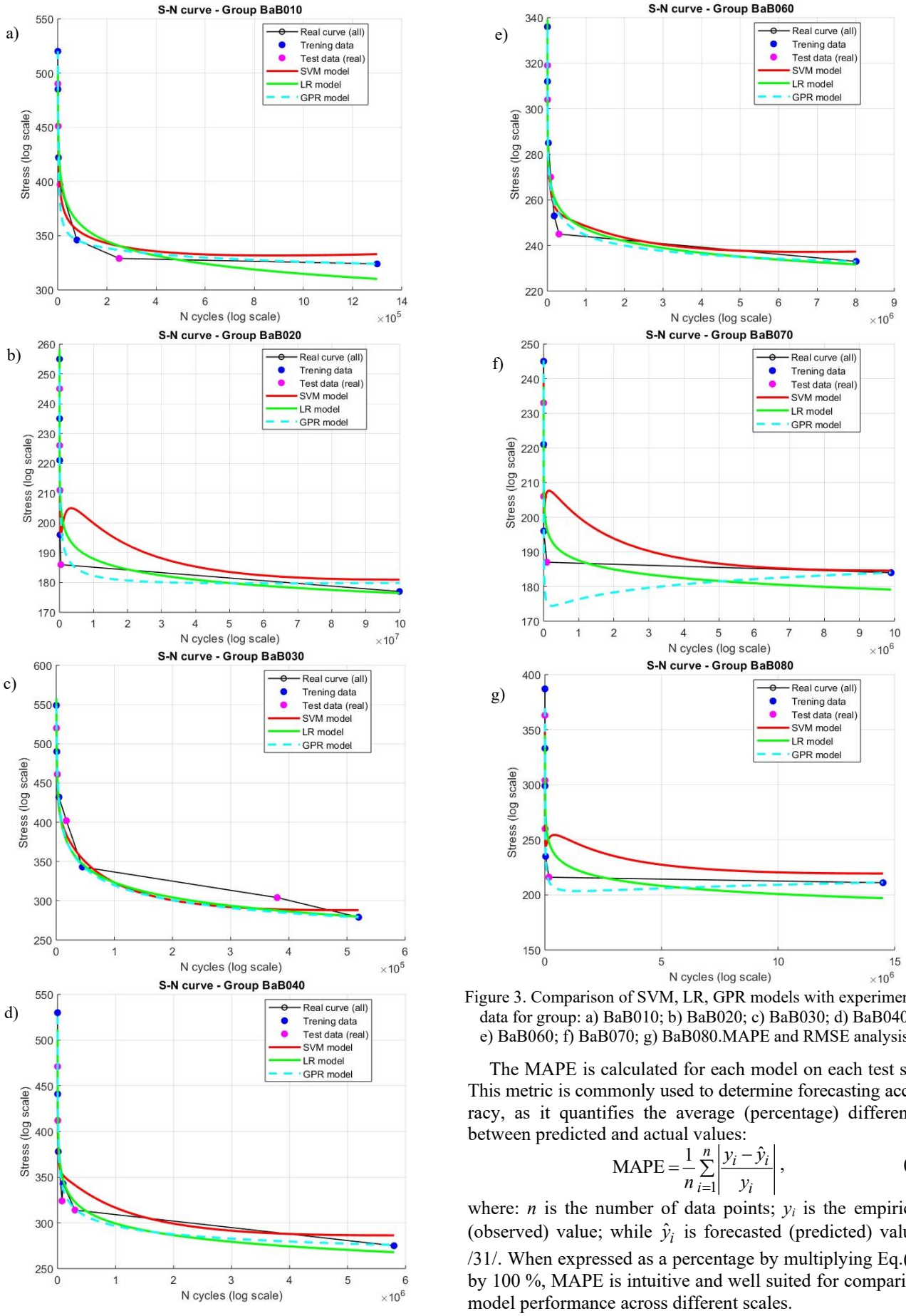

Figure 3. Comparison of SVM, LR, GPR models with experimental data for group: a) BaB010; b) BaB020; c) BaB030; d) BaB040; e) BaB060; f) BaB070; g) BaB080.MAPE and RMSE analysis.

The MAPE is calculated for each model on each test set. This metric is commonly used to determine forecasting accuracy, as it quantifies the average (percentage) difference between predicted and actual values:

$$\mathrm{MAPE} = \frac{1}{n}\sum_{i=1}^{n}\left|\frac{y_i - \hat{y}_i}{y_i}\right|, \tag{7}$$

where: n is the number of data points; y_i is the empirical (observed) value; while $\hat{y}_i$ is forecasted (predicted) value, /31/. When expressed as a percentage by multiplying Eq.(7) by 100 %, MAPE is intuitive and well suited for comparing model performance across different scales.

To evaluate the generalisation performance of applied models, the Root Mean Square Error (RMSE) method is also employed. Mathematically, RMSE is defined by the following expression:

$$\mathrm{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}\ . \tag{8}$$

Consequently, RMSE represents the standard deviation of the residuals, where residuals correspond to the stochastic differences between the regression line and observed data points, /31/. RMSE thus quantifies the dispersion of residuals, reflecting how closely the model's predicted values cluster around the observed values. Furthermore, it provides insight into the absolute magnitude of prediction errors.

Figure 4 shows the MAPE values across all valid groups for each model. The average MAPE values are: 4.17 % for SVM; 4.46 % for LR; 2.70 % for GPR.

Results of analysis for group BaB010 suggest that the SVM predictive curve shows excellent agreement with both training and test data. LR model also follows experimental trend closely, while the GPR predictions tend to slightly deviate from the actual data at low counts. MAPE values for SVM, LR, and GPR are 1.90 %, 1.96 %, and 3.11 %, in respect. Despite having a MAPE similar to SVM, LR exhibits limited ability to accurately follow the trend of the experimental curve, as illustrated in Fig. 3a. RMSE values for SVM, LR, and GPR are 9.02, 9.21, and 13.81, in respect. Calculations suggest that SVM model has the lowest MAPE and RMSE. LR approach is very close to SVM in terms of MAPE and RMSE. The GPR model exhibits the highest MAPE and RMSE values, indicating that it is the least accurate for this dataset.

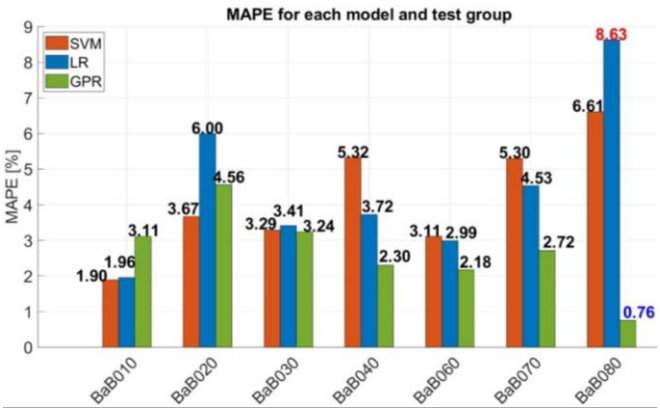

Figure 4. Comparison of MAPE for all experimental data.

As for the BaB020 group, SVM and GPR are suitable models, but LR is less reliable. MAPE values for SVM, LR, and GPR are 3.67 %, 6.00 %, and 4.56 %, respectively. RMSE values for SVM, LR, and GPR are 8.67, 15.43 and 12.13, respectively. Therefore, the SVM model is the most reliable for this group, performing best in terms of both MAPE and RMSE. The LR model is clearly too simplistic, and as a linear approach is insufficient for this dataset. The GPR model outperforms LR but falls short of SVM according to the performance metrics. Interestingly, as shown in Fig. 3b, although the SVM curve (red line) appears to deviate more from the actual curve than the GPR curve (blue dashed line), it still provides the most accurate predictions on average, as confirmed by the metrics used.

The results for group BaB030 indicate that all models fit well across the entire fatigue range, and GPR model and LR models follow the SVM model rather closely. MAPE values for SVM, LR, and GPR are 3.29 %, 3.41 %, and 3.24 %, respectively. Similarly, RMSE values for SVM, LR, and GPR are 13.51, 15.46, and 15.35, respectively. Among the models, SVM achieves both the lowest MAPE and RMSE, indicating that it produces the smallest average errors and provides the closest fit to the data.

For group BaB040, the GPR model provides the best fit, while the SVM and LR models show noticeable deviations from the observed data. The MAPE values are 5.32 % for SVM, 3.72 % for LR, and 2.30 % for GPR, and corresponding RMSE values are 20.90, 15.55, and 10.83, respectively. These results indicate that GPR delivers the most accurate predictions for this group, while the LR model ranks second, offering reasonable performance but lower predictive accuracy than GPR.

For group BaB060, the GPR model demonstrates strong generalisation and follows experimental training and test trend as well as LR and SVM models. MAPE values for SVM, LR, and GPR are 3.11 %, 2.99 %, and 2.18 %, in respect, while the corresponding RMSE values are 9.07, 9.03, and 6.28. The difference between SVM and LR is minimal, with LR performing slightly better, while GPR achieves the best overall results.

Interestingly, all three models for group BaB070 show deviations from experimental data; however, the GPR model provides the most accurate predictions. This is evidenced by MAPE values of 5.30 % for SVM, 4.53 % for LR, and 2.72 % for GPR, as well as RMSE values of 12.87, 9.54, and 7.08, respectively. The trend repeats, GPR model is the best predictive model in this group, while LR model would represent a suitable alternative.

Similar to the previous group, all three models show deviations for BaB080; however, GPR provides the best fit, with the lowest errors (MAPE = 0.76 %, RMSE = 2.38), compared to SVM (MAPE = 6.61 %, RMSE = 20.36) and LR (MAPE = 8.63 %, RMSE = 24.38). The GPR model demonstrates good accuracy, significantly outperforming the SVM and LR models, which exhibited higher error margins compared to previous groups.

DISCUSSION

For groups BaB040, BaB060, BaB070, and BaB080, the GPR model demonstrates the highest accuracy. It performs particularly well with nonlinear, smooth data and in cases where the relationship between input and output is complex. In the group BaB080 it particularly excels, suggesting that GPR is particularly suited for cases with pronounced nonlinearity. Also it is suitable for small or medium dataset sizes with smooth behaviour. The SVM model performs well when the data has a clear structure and less nonlinearity. In the BaB030 group it is very close to GPR, which means that it is still competitive when there are no large nonlinear jumps. The LR model is the weakest performer for BaB020 and BaB080 groups, which confirms that it is not robust to

nonlinearity. It performs adequately when data is close to linear behaviour (which is the case with BaB010, BaB030 and BaB060 groups) but quickly loses accuracy as soon as the patterns get more complex.

Overall, GPR achieves the lowest MAPE values, indicating that it provides the most accurate estimation of fatigue resistance based on the S-N curves overall and particularly for nonlinear S-N relationship. SVM exhibits higher MAPE values then GPR, but SVM still produces estimates of fatigue resistance that are useful. LR produces reasonable estimates of fatigue resistance on average, but it performs worse overall in terms of estimating the lower bound values initiated from groups with relatively low numbers of acceptable sample observations. In some cases, LR significantly exceeds experimental values, but overall, no MAPE value exceeds 10 %.

CONCLUSIONS

This investigation demonstrates the capability of the applied machine learning models (SVM, LR and GPR) to predict S-N curves based on experimental fatigue data. Among 3 models, GPR is the most reliable performer with the least MAPE values in most test groups, indicating its capacity to provide effective predictions for the nonlinear fatigue behaviour of the materials. The SVM model also shows strong performance and produces credible fatigue predictions for the available Ck35 dataset. Although LR is simple and easily interpretable, it can still serve as a reasonably effective method for characterising fatigue behaviour under appropriate conditions.

In summary, the application of advanced regression methods in conjunction with the Wöhler (S–N) curves developed from widely available data has potential to significantly increase the accuracy and reliability of fatigue life prediction. The advanced regression models are not only alternative to physical testing procedures but also provide an efficient and practical tool to support preliminary design studies.

As a part of future work, authors propose the application of other machine learning models as well as Artificial Neural Network and Deep Learning Algorithms.

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