Quest Journals
Journal of Software Engineering and Simulation
Volume 12 ~ Issue 5 (May 2026) pp: 14-18
ISSN(Online) :2321-3795 ISSN (Print):2321-3809
www.questjournals.org

Research Paper

Prediction of Fatigue Strength of Steel Materials Based on CoatiOA-LSSVMs

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Abstract
Steel fatigue strength is nonlinearly coupled with multiple influencing factors including chemical composition, heat treatment procedures and surface conditions, which makes it difficult to establish an accurate mechanistic model. To address this issue, this study proposes a prediction method combining coati optimization algorithm and least squares support vector machine (CoatiOA-LSSVM). The least squares support vector machine (LSSVM) is adopted to construct the mapping relationship between input variables and fatigue strength owing to its outstanding capability in fitting nonlinear data. The coati optimization algorithm (CoatiOA) is introduced to conduct global optimization for the regularization parameter γ and kernel width parameter σ of LSSVM, so as to eliminate the drawbacks of subjective parameter selection and local optimum trapping in manual tuning. Simulation experiments are carried out on a public steel fatigue strength dataset. The experimental results demonstrate that the proposed CoatiOA-LSSVM achieves lower root mean square error and higher coefficient of determination compared with the conventional LSSVM. It presents superior prediction accuracy and generalization performance, and can be applied to rapid fatigue strength prediction and process parameter optimization for steel materials.

Keywords*: steel materials, fatigue strength, least squares support vector machine (LSSVM), coati optimization algorithm (CoatiOA), prediction*

*Received 13 May., 2026; **R**evised 26 May., 2026; **A**ccepted 28 May., 2026 © The author(s) 2026.*
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I. Introduction

Steel materials are widely used in core equipment such as construction machinery, pressure vessels and rail transit facilities. Fatigue strength serves as a key performance indicator that determines the service life and operational safety of structural components. The fatigue performance of steel is affected by multiple factors, including chemical compositions (carbon, silicon, manganese, etc.), heat treatment temperature, holding time, cooling modes, surface roughness and stress ratio. These factors feature strong nonlinearity and complex coupling relationships, making traditional theoretical formulas incapable of accurately reflecting the underlying laws.

Current approaches for fatigue strength prediction mainly cover experimental testing, regression analysis, grey model, neural network, and support vector machine (SVM). The experimental method entails high costs and long testing cycles. Conventional statistical models have limited nonlinear fitting capacity, while single neural networks are prone to overfitting and perform poorly with small sample datasets. Following the principle of structural risk minimization, the least squares support vector machine (LSSVM) transforms the inequality constraints of standard SVM into equality constraints, and converts quadratic programming problems into linear equation systems. It features fast computation and excellent generalization ability, making it well-suited for nonlinear regression tasks with limited samples. Nevertheless, the prediction performance of LSSVM heavily relies on the selection of regularization parameter γ and kernel width σ. The manual trial-and-error parameter tuning method is inefficient and hardly yields the optimal parameter combination. To solve this problem, this paper adopts the coati optimization algorithm (CoatiOA) to intelligently optimize the core parameters of LSSVM, and establishes a CoatiOA-LSSVM model for steel fatigue strength prediction. A total of 437 groups of measured steel sample data are applied for model validation. The proposed method provides an effective solution for the intelligent prediction of steel fatigue strength[1], [2], [3], [4].

II. Relevant Theories and Model Construction

2.1 Principle of Least Squares Support Vector Machine

Least Squares Support Vector Machine (LSSVM) was proposed by Suykens and colleagues[5], [6]. It replaces the inequality constraints in standard SVM with equality constraints and converts quadratic programming into the solution of linear equation systems. This method greatly reduces computational complexity while retaining favorable generalization performance [7]. The core distinctions between LSSVM and conventional SVM lie in loss functions and constraint conditions. LSSVM adopts the quadratic term of error as its loss function, modifies the original inequality constraints into equality constraints, and thereby transforms the complicated convex quadratic programming problem into a simple linear equation solving task.

Let the training sample set of the model be $(x_i, y_i), i = 1,2, \dots, N$. Here, $x_i \in R^d$ denotes the d-dimensional input feature vector representing sample data of influencing factors for power load, and $y_i \in R$ stands for the one-dimensional actual value of load output. To achieve accurate regression of nonlinear data, LSSVM maps low-dimensional nonlinear samples into a high-dimensional linear feature space via the nonlinear mapping function φ(·), and then constructs a constrained optimization objective function as follows:

$$minJ(\omega, \xi) = \frac{1}{2}\omega^{\mathrm{T}}\omega + \frac{1}{2}\gamma \sum_{i=1}^{N} \xi_i^2 \text{ s.t.} y_i = \omega^{\mathrm{T}}\varphi(x_i) + b + \xi_i \quad (1)$$

where ω represents the weight vector in the high-dimensional feature space;$\xi_i$denotes the fitting error during model training; γ is the regularization parameter, which mainly balances the fitting accuracy and model complexity to prevent overfitting and underfitting; b refers to the model bias; $\varphi(\cdot)$stands for the nonlinear mapping function from the input space to the high-dimensional feature space.

To solve the above constrained optimization problem, Lagrange multipliers a_i are introduced to establish the Lagrangian function, which converts the constrained optimization into an unconstrained one for solution:

$$L(\omega, b, a_i, \xi_i) = \frac{1}{2}\omega^{\mathrm{T}}\omega + \frac{1}{2}\gamma \sum_{i=1}^{N} \xi_i^2 - \sum_{i=1}^{N} a_i(\omega^{\mathrm{T}}\varphi(x_i) + b + \xi_i - y_i) \quad (2)$$

According to the optimality conditions for extreme values, partial derivatives are calculated with respect to the weight vectorω , bias b and fitting error b respectively, and all partial derivatives are set to zero to eliminate intermediate variables ω and ξ_i. Combined with the Mercer kernel theorem, the kernel function $K(x, x_i) = \varphi^{\mathrm{T}}(x)\varphi(x_i)$ is adopted. The kernel trick transforms inner product operations in high-dimensional space into kernel function calculations in low-dimensional space, thereby avoiding the curse of dimensionality caused by high-dimensional computation. In this study, the radial basis function (RBF) kernel with favorable generalization performance and strong adaptability is selected, and its specific expression is given as follows:

$$K(x, x_i) = \exp\left(-\frac{\|x - x_i\|^2}{2\sigma^2}\right) \quad (3)$$

where σ denotes the kernel width parameter. It directly governs the mapping distribution characteristics of the sample space and affects the model's generalization ability.

By solving the optimized linear equation system, the optimal solutions of Lagrange multipliers $a_i$and bias b can be obtained. Finally, the regression prediction decision function of LSSVM is derived as follows:

$$y(x) = \sum_{i=1}^{N} a_i K(x, x_i) + b \quad (4)$$

The prediction performance of the LSSVM model is highly dependent on the values of the regularization parameter γ and kernel width parameter σ . The conventional manual trial-and-error method features strong randomness and low efficiency. It is difficult to acquire the optimal parameter combination, which may result in poor model fitting, low prediction accuracy and insufficient generalization capability. To address this parameter optimization issue, this paper applies the Coati Optimization Algorithm (CoatiOA) to perform global optimization for the core parameters of LSSVM.

2.2 Coati Optimization Algorithm (CoatiOA)

The Coati Optimization Algorithm (COA), proposed by Dehghani et al. in 2022, is a novel swarm intelligence optimization algorithm. It realizes the dynamic balance between global exploration and local exploitation by simulating the cooperative hunting behavior of coatis when attacking iguanas and their random escape strategies when encountering natural enemies [8].

CoatiOA mainly simulates two typical behaviors of coatis. The first is the global exploration during iguana hunting, which enables extensive search in the solution space to prevent missing the optimal solution. The second refers to the local exploitation when evading predators, which conducts fine search around the neighborhood of the optimal solution to improve optimization accuracy. This algorithm well balances global exploration and local exploitation, and effectively addresses the drawbacks of slow convergence and easy trapping into local optima existing in traditional optimization algorithms.

During algorithm iteration, the positions of the coati population are initialized first to construct the initial solution space. In the exploration phase, population positions are updated to expand the search scope and traverse potential optimal regions within the solution space. Afterwards, the exploitation phase performs refined search about the current optimal individual, so that the algorithm gradually converges to the global optimal solution.

In this work, the average mean square error of 5-fold cross-validation is adopted as the fitness function of CoatiOA. The parameter combination (C,γ) ofLSSVM is continuously updated via population iteration to minimize the prediction error, and the optimal hyperparameter configuration is ultimately obtained.The optimization objective function and constraint conditions are presented [4]as follows:

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2} \quad (5)$$

2.3 Construction of CoatiOA-LSSVM Model

The overall workflow of the proposed CoatiOA-LSSVM model for steel fatigue strength prediction consists of four modules: data preprocessing, adaptive hyperparameter optimization, model training and prediction evaluation. The detailed procedure is illustrated in Figure 1, and the specific steps are described as follows:

Data preprocessing: Normalize the original steel fatigue strength dataset to eliminate dimensional differences among various features, and divide the dataset into training set and test set at a fixed ratio.

Adaptive hyperparameter optimization: Initialize core parameters of the Coati Optimization Algorithm (CoatiOA), including population size and maximum iteration number. Map the kernel parameter σ and regularization parameter γ of LSSVM to individual position information. Take the average root mean square error (RMSE) of K-fold cross-validation as the fitness function. Update population positions iteratively via the foraging, movement, and vigilance mechanisms of CoatiOA, and globally search the parameter space to obtain the optimal hyperparameter combination that minimizes the objective function.

Model training: After iteration terminates, output the optimal hyperparameters $[\gamma, \sigma]$, substitute them into the LSSVM model, and complete the construction and training of the CoatiOA-LSSVM prediction model using the training set.

Prediction evaluation: Use the test set to conduct fatigue strength prediction with the trained model, and adopt indicators such as R^2, RMSE and MAE to evaluate model performance.

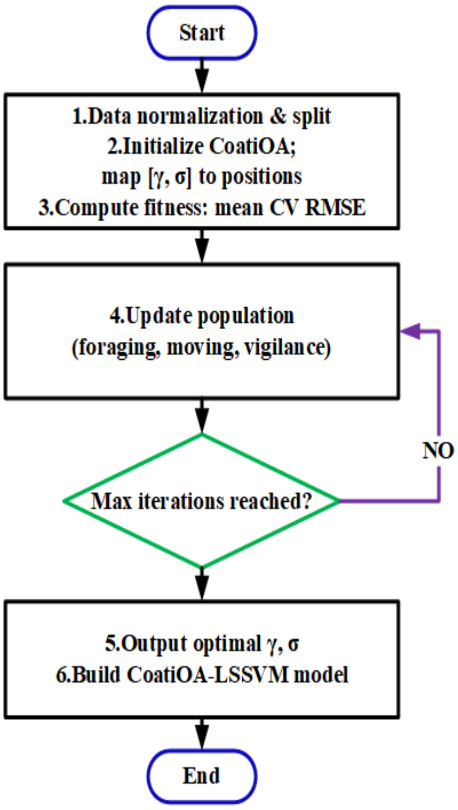

Fig.1 Flowchart of the proposedCoatiOA-LSSVM model for steel fatigue strength prediction

III. Experiments and Result Analysis

3.1 Dataset Overview

The steel fatigue strength dataset used in this study is sourced from the public dataset released by the National Institute for Materials Science (NIMS), Japan [9],[10]. It contains a total of 437 samples with 25-dimensional variables, including heat treatment parameters, cooling parameters, chemical compositions (C, Si, Mn, P, S, Ni, Cr, Cu, Mo), deformation parameters and steel fatigue strength values.

3.2 Experimental Settings

The coefficient of determination R^2, root mean square error (RMSE) and mean absolute error (MAE) are adopted as model evaluation metrics to verify the prediction accuracy and generalization ability of Coati Optimization Algorithm (CoatiOA) optimized least squares support vector machine (LSSVM). Comparative analysis is also conducted against the LSSVM model with default parameters.

In this experiment, 24-dimensional features are taken as inputs and steel fatigue strength as the output target. The optimized parameters are the regularization parameter γ and kernel parameter σ of LSSVM. The detailed experimental parameters are set as follows:

Parameter settings of CoatiOA: population size is 30, and the maximum number of iterations is 50.Parameter search range of LSSVM:

$$\gamma \in [1,1000], \sigma \in [0.01,10]$$

Model training settings: K-fold cross-validation is adopted($K = 5$) .

3.3 Analysis of Model Optimization Process

The iterative convergence curve of parameter optimization for LSSVM by CoatiOA is shown in Figure 2, which intuitively presents the variation trend of RMSE during algorithm iteration. The initial cross-validation RMSE of the algorithm is 119.3679 MPa. The optimization converges at a remarkably fast rate: the RMSE drops sharply to 26.0378 MPa after the first iteration. Accurate optimization continues in the first eight iterations, with the RMSE gradually converging to 25.4005 MPa. From the 8th to the 50th iteration, the optimal RMSE remains stable without fluctuation. The results demonstrate that CoatiOA possesses strong local search capability and rapid convergence performance. It can obtain the optimal parameter combination of LSSVM within a small number of iterations, and effectively overcome the drawbacks of traditional optimization algorithms, such as easy trapping in local optima and slow convergence.

After optimization, the optimal parameters of LSSVM are obtained as follows: regularization parameter $C = 441.917202$, kernel parameter $\gamma = 0.010599$, and the optimal cross-validation RMSE is 25.4005 MPa.

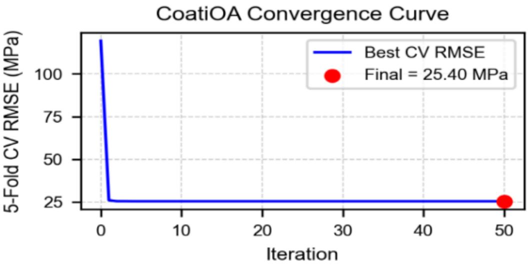

Fig.2 Convergence curve of the CoatiOA algorithm

3.4 Comparative Analysis of Model Prediction Performance

Experiments were conducted to test the steel fatigue strength prediction performance of the LSSVM with default parameters and the CoatiOA-LSSVM model. The results are presented in Table 1.

Table 1 Comparison of model prediction performance

Model	R^2	RMSE (MPa)	MAE (MPa)
Default LSSVM	0.8631	75.24	51.90
CoatiOA-LSSVM	0.9854	24.61	17.37
Performance Improvement	+0.1223	-50.63	-34.53

It can be seen from the quantitative results that:

The fitting accuracy is significantly improved. The coefficient of determination R^2 of the CoatiOA-LSSVM model reaches 0.9854, an increase of 0.1223 compared with the original LSSVM with default parameters. This indicates that the optimized model achieves an excellent fitting effect on steel fatigue strength and possesses much stronger capability in capturing data features.

The prediction error is greatly reduced. The RMSE of the optimized model is 24.61 MPa, which is 50.63 MPa lower than that of the default model. Its MAE is 17.37 MPa, a decrease of 34.53 MPa. Both core error indicators drop sharply, verifying that the prediction accuracy of the model is substantially improved.

Excellent generalization ability: CoatiOA finds the optimal hyperparameters through global optimization. It addresses the poor adaptability and weak generalization of LSSVM with default parameters, enabling the model to maintain high prediction accuracy on unseen test samples.

IV. Conclusion

Aiming at the problems of multi-factor coupling and complex nonlinear relationships in the prediction of steel fatigue strength, this paper proposes a prediction model combining the Coati Optimization Algorithm (CoatiOA) and Least Squares Support Vector Machine (LSSVM). CoatiOA is adopted to automatically determine the key parameters of LSSVM via its global optimization capability, which avoids the limitations of manual parameter tuning. Experiments are carried out on measured datasets, and the main conclusions are drawn as follows:

4.1High optimization efficiency of CoatiOA

CoatiOA can rapidly converge to the global optimum within a small number of iterations. It effectively addresses the parameter sensitivity issue of LSSVM, demonstrating excellent optimization efficiency and convergence stability.

4.2 The CoatiOA-LSSVM model achieves obviously higher accuracy than the original LSSVM with default parameters

After optimization by CoatiOA, the model presents substantial improvements in fitting accuracy and prediction error on the test set. Its performance is greatly enhanced compared with the original LSSVM with default parameters, which verifies the effectiveness and superiority of the proposed optimization strategy.

4.3 Possesses practical engineering application value

This model can accurately predict the fatigue strength of steel based on chemical compositions and processing parameters, and realize nonlinear mapping under multi-factor coupling. It provides a reliable data-driven tool for anti-fatigue material design, process optimization and service life evaluation.

Acknowledgments

This work was supported in part by the Project of PhDs' Start-up Research of GDUPT under Grant BS-XJ2022000501.

Guangdong University of Petrochemical Technology. Project No. 2019rc076. (702-519186, 702-71013303119, 702-72100003102, 702-72200010122, 702-72200010358; 71013407126, 71013407136, 7103513124128, 71013407130, 71013513124258, 24C258, 25B130, 25B131, 25C207,26B134,26C271,26C272).

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