Engineering Applications of Artificial Intelligence 133 (2024) 108270

Contents lists available at ScienceDirect

Engineering Applications of Artificial Intelligence

journal homepage: www.elsevier.com/locate/engappai

Research paper

Performance prediction and Bayesian optimization of screw compressors using Gaussian Process Regression

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A R T I C L E I N F O

Keywords:
Screw compressors
Gaussian Process Regression (GPR)
Bayesian optimization
Machine learning

A B S T R A C T

Optimizing the performance of screw compressors is critical for achieving high efficiency and reducing costs in various industrial and engineering applications. Often, the design and optimization processes are time-consuming owing to the underlying iterative complex analyses. In this context, the present research investigates the potential of Gaussian Process Regression (GPR) and Bayesian optimization for the prediction and optimization of the performance of an oil-flooded screw compressor. Specifically, the GPR-based surrogate model is developed to predict the compressor performance characteristics based on its four main geometrical design parameters such as wrap angle, relative length, tip speed of the male rotor and built-in volume ratio. The model is trained using a dataset comprising 19,200 data points relating the input design parameters with the compressor performance, obtained using physics-based multi-chamber thermodynamic models. While four different learning algorithms such as Support Vector Machine (SVM), Artificial Neural Network (ANN), Polynomial regression and GPR are explored, the GPR performed the best resulting in an R^2 value of 0.99 for the test dataset after hyperparameter tuning. Further, the model is also experimentally validated on a completely unseen dataset, showing very good predictions with a maximum error of 5%. The resulting surrogate model is then used to optimize the compressor design parameters using Bayesian optimization. The results are compared with optimization using Genetic Algorithm (GA) and physics-based multi-chamber thermodynamic model. It was shown the proposed approach results in similar optimal design parameters but with a significantly less optimization time by a factor of 7. The study highlight the potential of machine learning-based prediction and optimization of screw compressors in engineering applications.

1. Introduction

Compressors play a crucial role in numerous industrial and engineering applications, ranging from refrigeration and air conditioning systems to gas compression and processing plants.

As a consequence of their wider use, compressors consume 15%–20% of world electricity generation (Abdan et al., 2022). Amongst different types of compressors, screw compressors are particularly known for their compact design, relatively low noise levels, and the ability to deliver continuous, pulsation-free compressed air or gas. As a result, they are widely employed across various sectors, including the oil and gas, chemical, food processing, and power generation industries. To meet environmental concerns, every effort is, therefore, needed to improve their efficiency. Performance optimization is one way of enhancing efficiency and minimizing operating costs whereby one can reduce energy consumption, extend the equipment's lifespan, and lower maintenance expenses. In light of these factors, developing accurate and cost-effective methods for predicting and optimizing the performance of screw compressors is imperative for both industrial and engineering contexts.

The accurate prediction and optimization of screw compressor performance, particularly in relation to geometrical parameters, is important for both research and practical applications. Key geometrical parameters, such as the wrap angle of screw rotors (ϕ), relative length of rotors (L/D), tip speed of the male rotor (W_{tip}), and built-in volume ratio (VI), significantly influence the compressor's performance, efficiency, and operating range (Stosic et al., 2003). The complex interactions between these parameters and the nonlinear nature of the compression process make it difficult to establish precise relationships for performance prediction and optimization.

Existing methods for performance prediction and optimization of screw compressors typically involve empirical correlations, analytical

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https://doi.org/10.1016/j.engappai.2024.108270
Received 10 October 2023; Received in revised form 15 February 2024; Accepted 11 March 2024
Available online 22 March 2024

Nomenclature

ϕ	Wrap Angle of Screw Rotors
ETAK	Adiabatic Efficiency
GPR	Gaussian Process Regression
ML	Machine Learning
Q	Volume Flow Rate
R^2	Coefficient of Determination
SVM	Support Vector Machine
VI	Built-in Volume Ratio
ANN	Artificial Neural Network
GA	Genetic Algorithm
L/D	Relative Length of Rotors
P	Power Consumption
RMSE	Root Mean Squared Error
SCORG	Screw Compressor Rotor Grid Generation
W_{tip}	Tip Speed of the Male Rotor
ETAV	Volumetric Efficiency

models, or numerical simulations. Empirical correlations, derived from experimental data, are often limited in their applicability due to the specificity of the test conditions and compressor configurations. Analytical models, on the other hand, are based on simplifying assumptions that may not accurately represent the complex behavior of real-world compressors, particularly when considering critical geometrical parameters (Stosic et al., 2005). Finally, numerical simulations, such as Computational Fluid Dynamics (CFD) (Kovacevic et al., 2016), can provide detailed insights into the compressor performance but often require significant computational resources and time, making them less practical for real-time optimization and control. These limitations highlight the need for a novel approach that can efficiently and accurately predict the performance of screw compressors and simultaneously facilitate effective optimization in a computationally efficient manner. In this context, Machine Learning (ML) approaches have gained significant attention recently in the engineering research community as a potential alternative to assist the design, performance estimation (Marx et al., 2018) and optimization process (Joly et al., 2019). While a range of ML architectures are proposed and further utilized in a range of engineering applications, Gaussian Process Regression (GPR) (Melo, 2012) is found to be an appropriate choice for predictions due to its probabilistic approach to regression. Essentially, GPR models the underlying function as a Gaussian process, allowing it to capture complex relationships between input variables and output responses together with quantifying the uncertainties in the predictions. It has garnered significant interest in recent years particularly when compared to other methods such as Support Vector Machines (SVM) (Salcedo-Sanz et al., 2014; Ying et al., 2020), Artificial Neural Networks (ANN) (Krogh, 2008), and polynomial regression (Staudenmayer and Ruppert, 2004). The strength of GPR lies in its ability to provide both a predictive mean and an uncertainty estimate, offering valuable insights into the underlying structure of data.

In this present study, various machine learning models, including Support Vector Machines, Artificial Neural Networks, polynomial regression, and Gaussian Process Regression, were considered for the performance prediction of screw compressors. The results indicated that GPR outperformed the other models in terms of accuracy and its inherent uncertainty quantification, making it the most suitable choice for the present application. Further in this study, Bayesian optimization was employed to tune the hyperparameters of the GPR model, further enhancing its performance prediction capabilities. The Bayesian optimization technique leverages probabilistic models, such as the Gaussian processes, to construct a surrogate model of the objective function, which is then used to guide the search for the optimal solution. One of the key advantages of Bayesian optimization is its ability to balance exploration and exploitation in the search process, enabling it to effectively navigate the optimization landscape.

Some of the earliest studies on Bayesian interpolation, regression and classification are from MacKay (1992) and Gibbs (1998). This technique has been recently deployed very successfully to solve various regression and classification problems in multiple disciplines of engineering (Ma et al., 2023; Yadav et al., 2023; Zhao et al., 2022, 2023b; Morita et al., 2022; Kopsiaftis et al., 2019; Richardson et al., 2017; Sterling et al., 2015; Injadat et al., 2018). Bayesian optimization has found applications in materials design through experiment guidance via Gaussian process regression (Frazier and Wang, 2015), as well as in crystal structure prediction using Bayesian techniques as a selection-type algorithm (Yamashita et al., 2018). An example of using GPR for validation of a physics-based vehicle dynamics model can be found in Rhode (2020). Several other machine learning approaches have been employed for a variety of engineering problems ranging from material property predictions (Nakka et al., 2023; Pathan et al., 2019; Fontes and Shadmehri, 2023) to structural health and condition monitoring (Rahbari et al., 2021; Liu et al., 2023; Zhao et al., 2023a), fault-tolerant control (Stojanović, 2023; Wang et al., 2023b; Deng et al., 2022) and manufacturing (Wuest et al., 2016).

In the domain of compressor systems, few studies exist, for instance, an artificial intelligence approach using neural networks has been used for optimizing the compressor scheduling process (Nguyen and Chan, 2006), fault diagnosis and severity assessment (Kim and Li, 1995) and predicting the operability of damaged compressors (Taylor et al., 2020). In Ghorbanian and Gholamrezaei (2009), an artificial neural network is used for compressor performance prediction. Specifically in screw compressors, Patil et al. (2022) shows a study on training artificial neural networks for predicting certain rotor profile characteristics and optimization (Wang et al., 2023a). While all the above studies have demonstrated the potential applications of AI-based approaches for engineering applications, very few studies exist in developing AI-based performance prediction and optimization models in the context of compressor systems. The performance characteristics are hitherto determined based on physics-based models (Stosic and Hanjalic, 1994; Analysis, 2014; Ziviani et al., 2020). From this perspective, the present work aims to develop an AI-assisted performance prediction and optimization framework using GPR and Bayesian algorithms. While various machine learning models, including Support Vector Machines (SVM), Artificial Neural Networks (ANN), and polynomial regression, have been utilized in performance prediction, none of these approaches have fully capitalized on the advantages offered by GPR, such as the uncertainty quantification and its adaptability to complex, nonlinear relationships. The proposed approach differs from previous studies in that it not only applies GPR for performance prediction but also leverages Bayesian optimization for hyperparameter tuning, further enhancing the model's capabilities.

A key research question addressed in the work is as follows: Can machine learning-based surrogate models accelerate the otherwise time-consuming performance prediction and optimization process in compressor systems, while providing accuracy and uncertainty estimates? In this regard, the contributions of this research are articulated below:

1. Introduction of a Gaussian Process Regression (GPR) surrogate model, trained on a comprehensive dataset, offering a computationally-efficient method for predicting oil-flooded screw compressor performance with very good accuracy.
2. Implementation of Bayesian optimization as an efficient algorithm for optimization of the compressor system, demonstrating a seven-fold reduction in optimization time compared to the Genetic Algorithm, thereby enhancing the computational efficiency of the optimization process.

Table 1
Key geometrical parameters considered for data set generation. Wrap angle of screw rotors (ϕ) in radians, relative length of rotors (L/D), tip speed of the male rotor (W_{tip}) in m/s, and built-in volume ratio (VI) are varied to generate diverse data sets.

Input parameters	Range	Step length	No. of instances
W_{tip} (m/s)	(15, 50)	0.7	50
VI	(2.1, 5.1)	0.5	6
L/D	(0.5, 2.5)	0.5	4
ϕ (rad)	(3.8, 7)	0.16	20
Total no. of data sets			24,000

3. Experimental validation of the GPR model on previously unseen data, establishing its reliability with very low prediction error. This validation underscores the model's robustness and generalization capabilities for real-world applications.

The paper is organized as follows: Section 2 summarizes the dataset generation procedure followed in this work. This is then followed by the development and training of GPR model using Bayesian hyperparameter tuning in Section 3. In this section, the discussion of prediction results together with uncertainty quantification especially on the extraterritorial predictions are presented. Section 4 presents the experimental validation of the GPR predictions on unseen data comprising the input parameters that are not seen by the model during training. Optimization of compressor design parameters is conducted in Section 5 using Bayesian optimization together, showcasing the computational efficiency of the proposed framework in comparison with the genetic algorithm, another commonly used evolutionary optimization technique. Concluding remarks are provided in Section 6.

2. Dataset generation

To effectively train a machine learning model, a large number of datasets are usually necessary depending on the application and the range of parameters involved. However, the acquisition of such a substantial dataset from experimental testing is often unfeasible. To address this challenge, a validated physics-based screw compressor model was developed and utilized in the present study. The screw compressor was modeled using SCORG (Screw Compressor Rotor Grid Generation) software from PDM Analysis, a leading grid generation and performance software for positive displacement screw machines. SCORG performs thermodynamic calculations based on a multi-chamber model, employing conservation equations of mass and internal energy for control volumes (Analysis, 2014; Stosic et al., 2005). The screw compressor considered in this study is the KAS-300 oil-flooded air screw compressor (gear-driven) with a built-in volume ratio of 4.6, operating at pressure ratios of 6.5, 8.5, 10.5, and 12.5, with a tip speed ranging from 15 to 45 m/s. It is manufactured by Kirloskar Pneumatic Company Limited in Pune, India. Due to its commercial nature, detailed information about the compressor's size and profile cannot be disclosed. Experimental testing for this compressor was conducted at the Centre for Compressor Technology, City University of London, and the obtained data was used for validating the screw compressor model in SCORG.

After setting up the SCORG model for this compressor configuration, a batch file was linked with the programming language, Python to automate the data generation framework. Four key design variables were selected to be varied within the data generation framework, and their respective ranges and step lengths are provided in the accompanying Table 1. This approach facilitated the generation of an extensive dataset comprising 24,000 individual instances.

To facilitate the interpretation and development of the machine learning model, heatmaps (Fig. 1) were generated for data set visualization. These heatmaps depict the correlations among the input variables and four key output parameters: Power Consumption (P), Volume Flow Rate (Q), Volumetric Efficiency (ETAV), and Adiabatic Efficiency (ETAK). These output parameters collectively define the compressor's

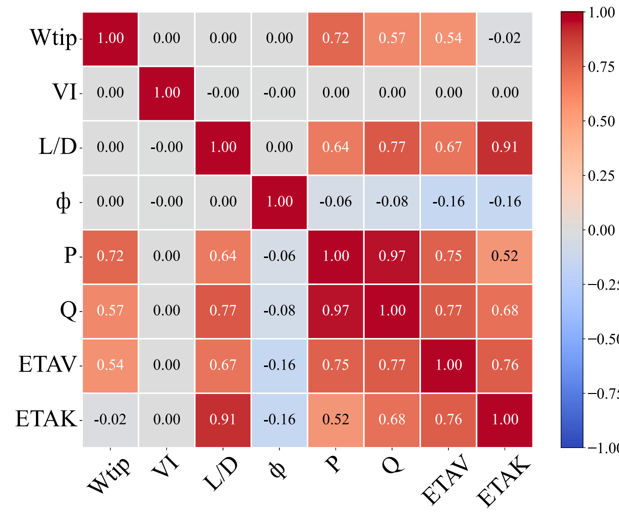


Fig. 1. Correlation Heatmaps illustrating the relationships between input parameters and key output parameters. Brighter colors represent more pronounced positive or negative correlations, while darker colors suggest weaker or negligible correlations.

operational effectiveness and energy efficiency. Power Consumption and Volume Flow Rate are direct indicators of the compressor's performance, representing the energy consumed and the amount of gas delivered at required pressures, respectively. Volumetric Efficiency (ETAV) is the ratio of actual to theoretical flow, reflecting the compressor's ability to deliver the expected gas volume. Adiabatic Efficiency (ETAK) is the ratio of theoretical to actual power consumption, indicating the efficiency with which the compressor converts power into useful work. Brighter colors in the heatmaps represent more pronounced positive or negative correlations, while darker colors suggest weaker or negligible correlations.

From Fig. 1 it is observed that the correlation values between the input variable "VI" (Built-in Volume Ratio) and the output parameters are consistently zero. This outcome is expected and can be attributed to the experimental nature of the dataset, where the variation in the Built-in Volume Ratio was intentionally kept constant for this specific set of experiments. Therefore, the lack of correlation with the output parameters aligns with the experimental design. On the other hand, the correlation values for other input variables such as W_{tip} (Tip Speed), L/D (Relative Length), and ϕ (Wrap Angle) exhibit varying degrees of correlation with the output parameters. Notably, the correlation values are indicative of the influence of these geometric parameters on compressor performance. The interpretation of these correlation heatmaps is essential for understanding the dataset and guiding the subsequent machine learning model development, contributing to the interpretability of the overall methodology.

3. Model development

3.1. Model architecture

Gaussian Process Regression (GPR) (Melo, 2012) is utilized as the primary governing machine learning model in this study. Unlike conventional regression techniques, GPR does not assume fixed functional forms for the data, rendering it suitable for handling complex and nonlinear relationships. The underlying concept of GPR relies on Gaussian processes and collections of random variables. The target variable is modeled as a multivariate Gaussian distribution, where the mean function represents the underlying trend, and the covariance function captures data uncertainty or noise. GPR provides both point predictions and predictive uncertainties, enabling robust decision-making and uncertainty quantification. The capability of GPR to handle uncertainty

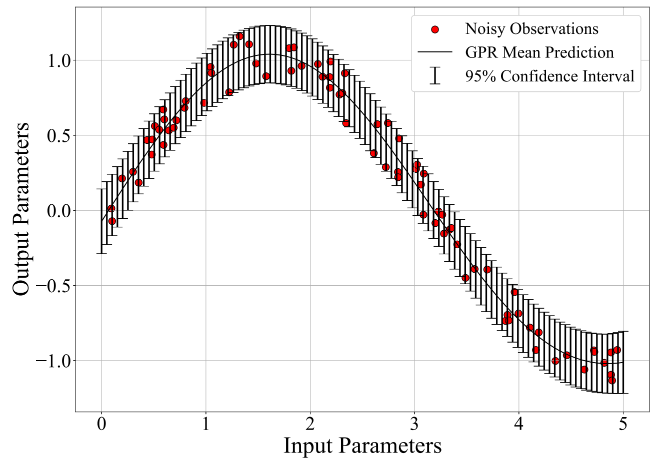


Fig. 2. Illustration of the inherent benefit of Gaussian Process Regression (GPR) as a surrogate model. The plot represents GPR mean prediction (black line) fitted to noisy observations (red dots) with indicated 95% confidence interval. This visual representation emphasizes GPR's unique ability to quantify prediction uncertainty.

is particularly advantageous in the current application, where accurate predictions and confidence intervals are vital for reliable compressor performance estimation.

Fig. 2 provides an example schematic of GPR model predictions (black line) fitted to noisy data, demonstrating its ability to estimate uncertainty through the shaded 95% interval.

Given a training dataset $\mathcal{D} = \{(\mathbf{x}_i, y_i)\}_{i=1}^{N}$ with input vectors $\mathbf{x}_i \in \mathbb{R}^d$ and corresponding outputs $y_i \in \mathbb{R}$, the goal of GPR is to predict the output y_* for a new input vector $\mathbf{x}_*$. The predicted output y_* is modeled as a Gaussian distribution:

$$y_* \sim \mathcal{N}(\mu_*, \sigma_*^2) \tag{1}$$

The mean μ_* and variance σ_*^2 of the predictive distribution are given by:

$$\mu_* = \mathbf{k}_*^\top (\mathbf{K} + \sigma_n^2 \mathbf{I})^{-1} \mathbf{y} \tag{2}$$

$$\sigma_*^2 = k(\mathbf{x}_*, \mathbf{x}_*) - \mathbf{k}_*^\top (\mathbf{K} + \sigma_n^2 \mathbf{I})^{-1} \mathbf{k}_* \tag{3}$$

where $\mathbf{k}_*$ is the vector of covariances between the training data and the new input vector, $\mathbf{K}$ is the covariance matrix of the training data, σ_n^2 is the noise variance, and $\mathbf{y}$ is the vector of training outputs. The choice of covariance function (kernel) $k(\cdot,\cdot)$ plays a crucial role in GPR, allowing flexibility in capturing different data relationships.

In addition to the GPR model, several other machine learning algorithms such as Support Vector Machines (SVM), Artificial Neural Networks (ANN), and polynomial regression, were also explored to assess their performance and suitability for the given task. Briefly, these algorithms are summarized below for completeness. SVM (Noble, 2006), a widely used supervised learning algorithm, seeks the optimal hyperplane that best separates data points of different classes in a high-dimensional space. SVM is suitable for both classification and regression tasks and offers strong generalization capabilities. ANN (Krogh, 2008) comprises interconnected nodes (neurons) organized in layers. It is a powerful deep learning technique capable of capturing complex relationships between input and output variables. Polynomial Regression (Wetherill and Wetherill, 1981) extends the traditional linear regression by fitting a polynomial function to the data. It is particularly useful when the relationship between the variables appears to be non-linear. The degree of the polynomial is a hyperparameter that can be tuned for improved model performance.

While each of these algorithms offers unique strengths and has been widely used in various domains, GPR demonstrated superior performance in terms of predictive accuracy and uncertainty quantification,

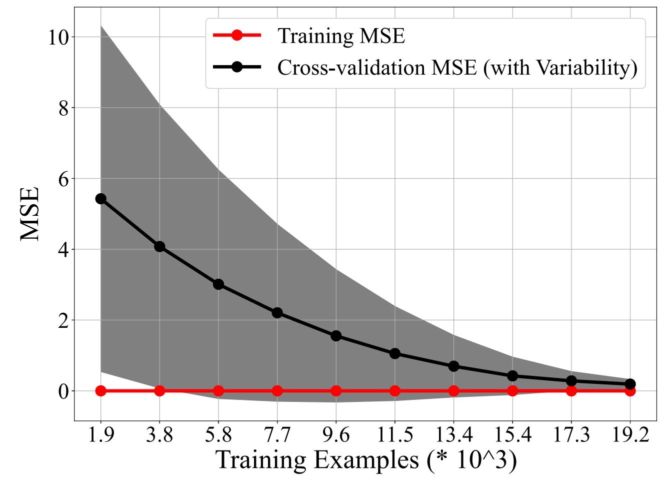


Fig. 3. Optimal dataset size for GPR model: Assessment of model performance with respect to training dataset size. The GPR model demonstrated optimal performance with a dataset size of 19,200, selected through initial optimization out of the total 24000 datasets. Increasing the dataset size beyond this point showed marginal impact on Mean Squared Error (MSE).

making it the preferred choice for the specific compressor performance estimation task in this study.

3.2. Dataset size optimization through initial training

The datasets generated for training machine learning (ML) models are often extensive, rendering them unsuitable for direct use in training due to the risk of overfitting or underfitting. Overfitting occurs when the model performs exceptionally well on the training data but poorly on unseen data, while underfitting arises when the model fails to capture the underlying patterns in the training data, leading to poor performance on both training and new data instances.

To address these concerns, a robust methodology was employed to determine the optimal quantity of data required for training the ML model, effectively avoiding overfitting and underfitting. This involved a detailed statistical and computational approach, which is elaborated below.

3.2.1. Methodology for determining dataset size

The process of determining the most suitable dataset size involved a combination of statistical and computational techniques. Initially, the Gaussian Process Regression (GPR) model was selected as the base model for assessing the effect of the dataset size on prediction accuracy.

A learning curve, as depicted in Fig. 3, was employed to analyze the model's performance. The x-axis represents the number of training examples, while the y-axis displays the mean squared error (MSE) as the performance metric. This visual representation provided insights into both the training and cross-validation performance of the model.

Furthermore, the statistical significance of the chosen dataset size was ensured through a comprehensive cross-validation approach, utilizing a 5-fold cross-validation strategy. This not only assessed the model's generalization capability but also provided insights into the variability in performance across different folds.

Alternative methodologies were considered during the optimization process. However, the selected approach demonstrated superior performance and stability in determining the optimal dataset size for training. The decision to exclude certain alternative methodologies was based on a careful evaluation of their suitability for the specific characteristics of the dataset and the overarching goals of the study.

In summary, the methodology for determining the dataset size involved a thoughtful combination of statistical techniques, computational analysis, and cross-validation strategies. The selected approach

Table 2
Comparison of Machine Learning models based on initial hyperparameter tuning for model selection. Root Mean Squared Error (RMSE) and Coefficient of Determination (R^2) are used to evaluate model performance.

ML models	RMSE	R^2 (%)
Training result		
SVM	0.2455	76.4566
ANN	0.1642	85.8493
Polynomial	0.2111	79.9818
GPR	0.1532	87.3984
Testing result		
SVM	0.2668	70.2781
ANN	0.1952	82.5561
Polynomial	0.2556	78.1888
GPR	0.1843	82.4344

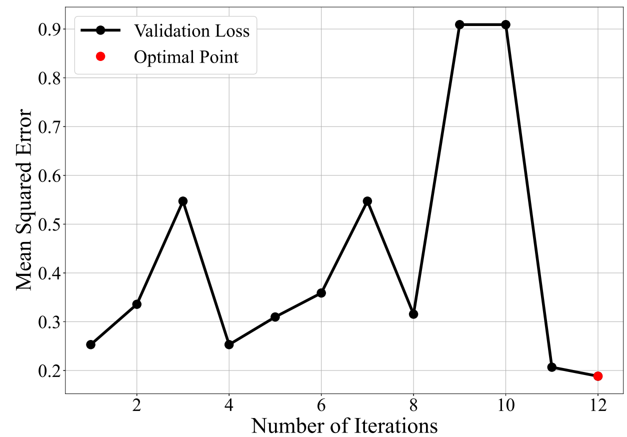


Fig. 4. Validation loss during hyperparameter tuning of GPR model with Bayesian optimization. The red dot indicates the optimal point where validation loss is minimized, yielding the optimal set of hyperparameters. The tuned model exhibits improved performance, reflected in a significant reduction in RMSE and increased R-squared values for both training and testing data.

was found to be robust, providing a foundation for ensuring the model's accuracy and generalization capabilities.

The GPR model, employed as the foundational model in this context, exhibited optimal performance with a dataset size of 19,200, derived from the initial optimization process out of the total dataset of 24000. Beyond this point, increasing the dataset size does not significantly alter the Mean Squared Error (MSE). The attained optimal MSE of 0.19035 underscores the model's precision in predicting the target variable based on the selected features. This finding suggests that a dataset size of 19,200 is sufficient for training the model, providing an optimal balance between accuracy and computational efficiency. This approach not only streamlines the training process but also conserves valuable computational resources, making it a judicious choice for practical implementation and model development.

Having arrived at the optimal size of the dataset, the next section will present the results of the four different ML models (including GPR), followed by further hyperparameter tuning of the best-performing model, which in the current case was the GPR.

3.3. Model training

In this section, all machine learning (ML) models based on initial hyperparameter tuning, including Gaussian Process Regression (GPR), were trained using the total dataset size of approximately 24000 instances obtained from Section 3.2. Out of the total dataset, 80% of instances were utilized for training the ML models, and the remaining 20% were reserved for testing. After training, the performance of each model was evaluated using the Root Mean Squared Error (RMSE) and the coefficient of determination (R^2) on both training and testing data. The results are summarized in Table 2.

From the table, it is evident that GPR outperforms all other ML models in both the training and testing phases. The GPR model exhibits the lowest RMSE values and highest R^2 percentages, indicating superior predictive accuracy and better fit to the data. The lower RMSE signifies the smaller average prediction error of the GPR model, while the higher R^2 indicates that a larger proportion of the target variable's variance is explained by the model. The subsequent subsection will focus on further hyperparameter tuning of the GPR model to further optimize its performance and ensure optimal generalization capabilities in real-world applications.

3.4. Hyperparameter tuning with optimal dataset size

In this section, a comprehensive insight is provided into the intricacies of the hyperparameter tuning process for the Gaussian Process Regression (GPR) model using the optimal dataset size of approximately 19,200 instances as evident from Section 3.2. The GPR model, chosen for its probabilistic and non-parametric regression capabilities, relies on kernel functions to adeptly capture intricate relationships within the dataset. The approach involves the utilization of the Radial Basis Function (RBF) kernel in conjunction with the White Kernel.

The RBF kernel, alternatively known as the squared exponential or Gaussian kernel, proves highly effective in capturing smooth variations within the underlying function. Its definition incorporates a length scale parameter, finely controlling the extent of influence for each data point. Additionally, the White Kernel introduces a noise term, crucial for accommodating the inherent uncertainties present in the data. This careful selection of kernels aligns seamlessly with the objective of precisely modeling the performance characteristics of screw compressors. Given the inherently non-linear and uncertain nature of these relationships, the chosen kernels contribute significantly to the model's accuracy.

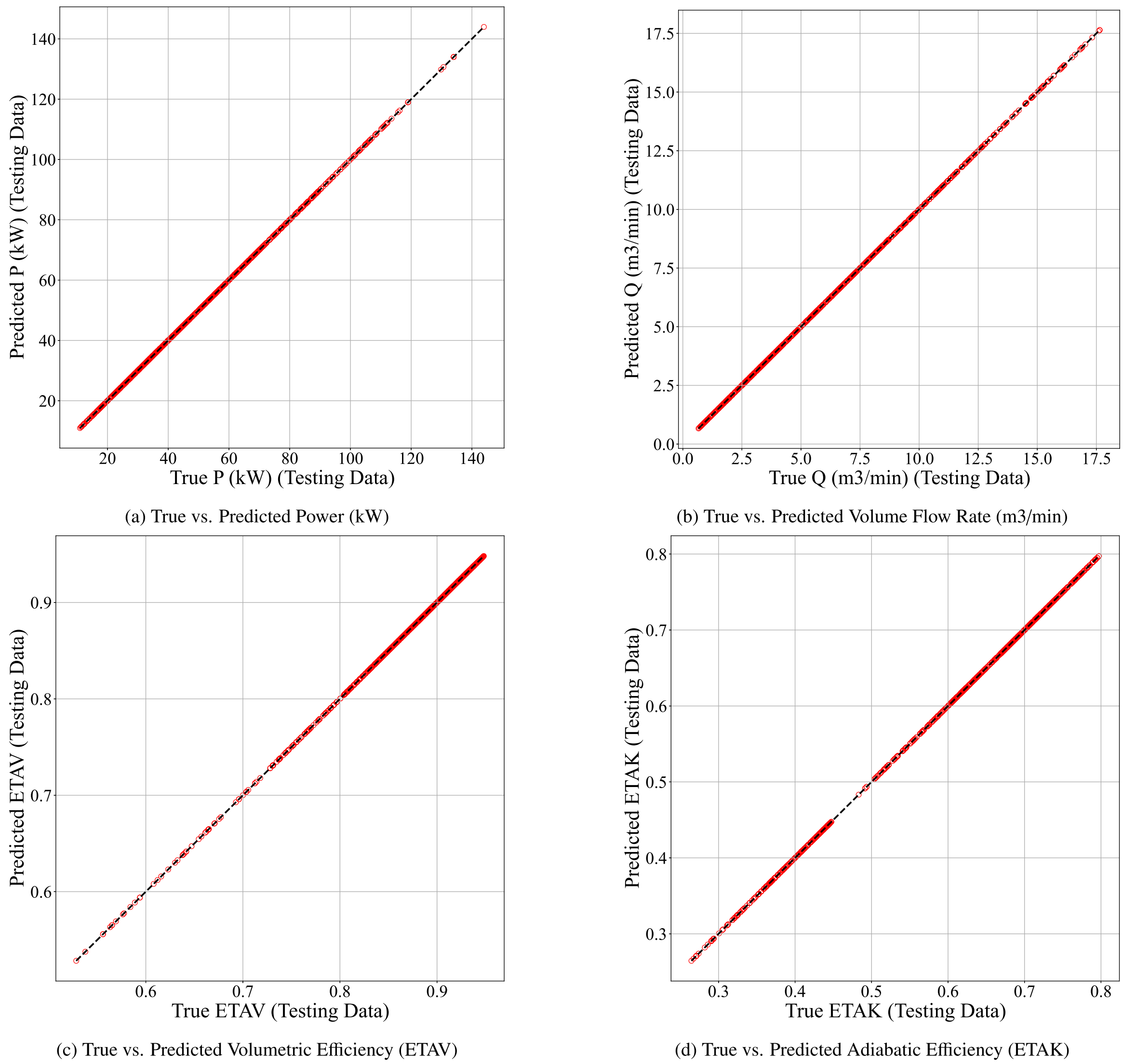
The hyperparameter tuning methodology employed in this study is centered around Bayesian optimization. Renowned for its efficiency in exploring the hyperparameter space with a minimal number of iterations, Bayesian optimization allows us to fine-tune specific parameters. In particular, the length scales of the RBF kernel and the noise level of the White Kernel are the focal points of optimization. The objective is to maximize the model's log marginal likelihood, thereby enhancing its overall fit to the training data.

Performance metrics, including Root Mean Squared Error (RMSE) and R-squared, are calculated for both training and testing datasets during the optimization process.

The Bayesian optimization process is mathematically described by the equation:

$$x_{\text{next}} = \arg\max_{x} \alpha(x) \cdot \mathcal{U}(x; \min, \max) \quad (4)$$

Where x_{next} represents the variable denoting the next point or input to be selected for evaluation in the optimization process. It is typically a vector in the input space. $\arg\max$ symbol is used to find the argument (in this case, the value of x) that maximizes the expression following it. It means we are looking for the input x that maximizes the acquisition function $\alpha(x) \cdot \mathcal{U}(x; \min, \max)$. $\alpha(x)$ represents the acquisition function. The choice of the acquisition function depends on the specific Bayesian optimization algorithm being used. Common choices include Expected Improvement (EI), Probability of Improvement (PI), and Upper Confidence Bound (UCB). The acquisition function quantifies the utility of evaluating the objective function at a particular input x. It guides the search by balancing exploration (trying new points) and exploitation (focusing on promising points). $\mathcal{U}(x; \min, \max)$ represents a probability



(a) True vs. Predicted Power (kW)

(b) True vs. Predicted Volume Flow Rate (m3/min)

(c) True vs. Predicted Volumetric Efficiency (ETAV)

(d) True vs. Predicted Adiabatic Efficiency (ETAK)

Fig. 5. Hyperparameter-tuned GPR model predictions for the compressor performance characteristics on the test dataset: Parity plots.

distribution over the input space. In Bayesian optimization, it is often used to model uncertainty or exploration. The notation $\mathcal{U}(x; \min, \max)$ typically denotes a uniform distribution over the input space, where min and max represent the minimum and maximum bounds for the input variables. This distribution encourages exploration within the specified bounds.

In summary, the equation describes how Bayesian optimization selects the next input point x_{next} by maximizing the acquisition function $\alpha(x)$ while considering a probability distribution $\mathcal{U}(x; \min, \max)$ that guides the exploration of the input space. The goal is to find the input x that is expected to yield the most valuable information for optimizing the objective function.

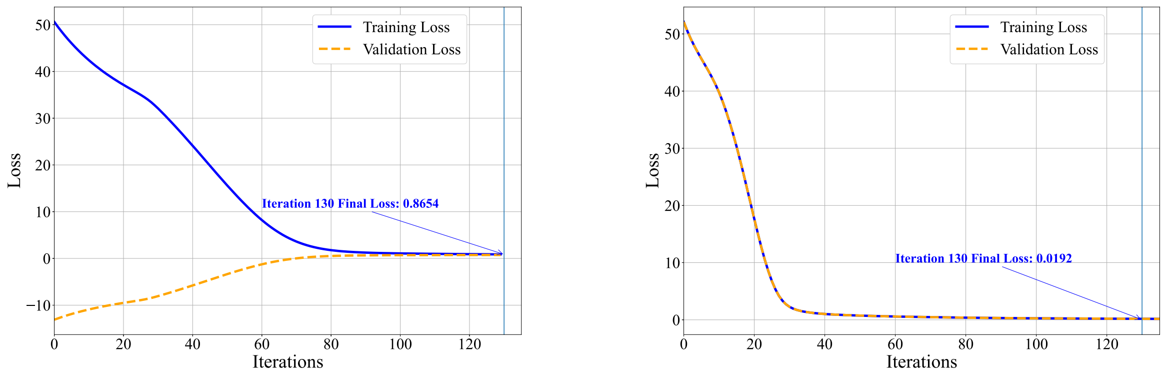
Fig. 4 shows the validation loss (mean squared error) of the GPR model during hyperparameter tuning using Bayesian optimization. The red dot represents the optimal point where the validation loss is minimized, leading to the optimal set of hyperparameters for the model. The tuned model demonstrates improved performance, evident from the substantial reduction in RMSE and the increase in R-squared values for both training and testing data. Visual comparisons of true vs. predicted values are presented in terms of parity plots in Fig. 5.

Fig. 6 shows the progression of training and validation loss over iterations for a GPR model before and after hyperparameter tuning. In Fig. 6(a), the model's initial performance without hyperparameter tuning is depicted. In Fig. 6(b), the effects of hyperparameter tuning on the model's convergence are demonstrated. The dashed orange line represents validation loss, the solid blue line indicates training loss and the red dotted line marks the point of early stopping. The optimized hyperparameters are listed in Table 3. The GPR model's performance shows significant enhancement, thereby providing more accurate predictions (Table 4). This hyperparameter-tuned GPR model will be further utilized to optimize screw compressor parameters, with the ultimate goal of reducing specific power consumption.

Table 3
Optimization of hyperparameters: Kernel Length Scale and Noise Level. The table depicts the search ranges and optimal values for the kernel length scale and noise level, highlighting the optimized hyperparameters for enhanced GPR model performance.

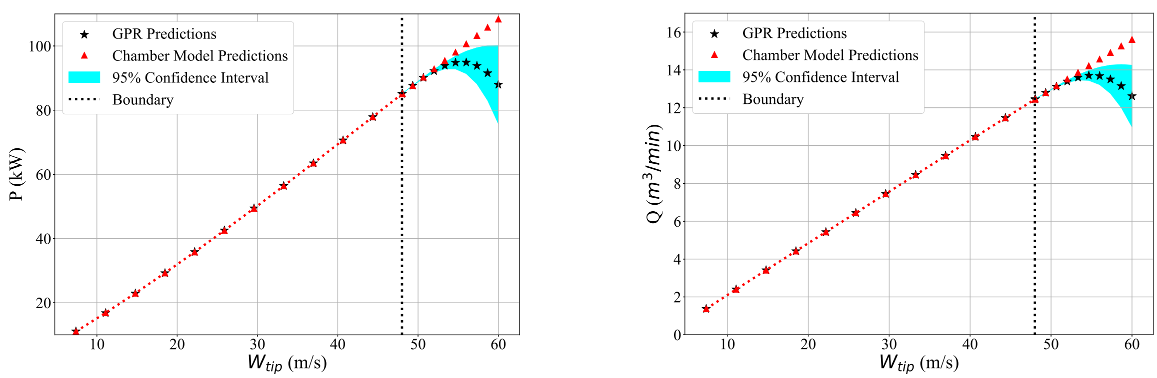
Hyperparameter	Range	Optimal value
Kernel Length Scale	(0.01, 10)	(8.4244, 8.8499, 7.4057, 6.3108)
Kernel Noise Level	(0.01, 100)	7.6409

Figs. 7, 8, 9, 10 illustrate the application of Gaussian Process Regression (GPR) as a surrogate model to perform predictions of the compressor performance characteristics as a function of tip speed (W_{tip}), built-in volume ratio (VI), relative length (L/D) & wrap angle (ϕ). From the prediction results, it is clear that the GPR model was able to capture the complex nonlinear relationship between the output and

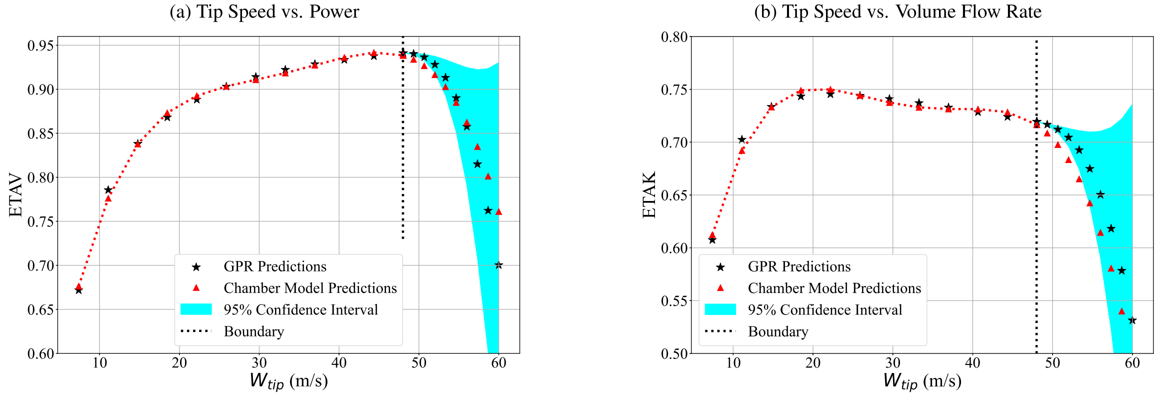


(a) Before hyperparameter tuning (b) After hyperparameter Tuning

Fig. 6. Learning curve of the GPR model before and after hyperparameter tuning. The plot illustrates the convergence of the GPR model with the number of iterations during training. After hyperparameter tuning, the final loss significantly decreased from 0.8654 to 0.0192 at the 130th iteration, indicating improved model convergence and predictive performance.



(a) Tip Speed vs. Power (b) Tip Speed vs. Volume Flow Rate



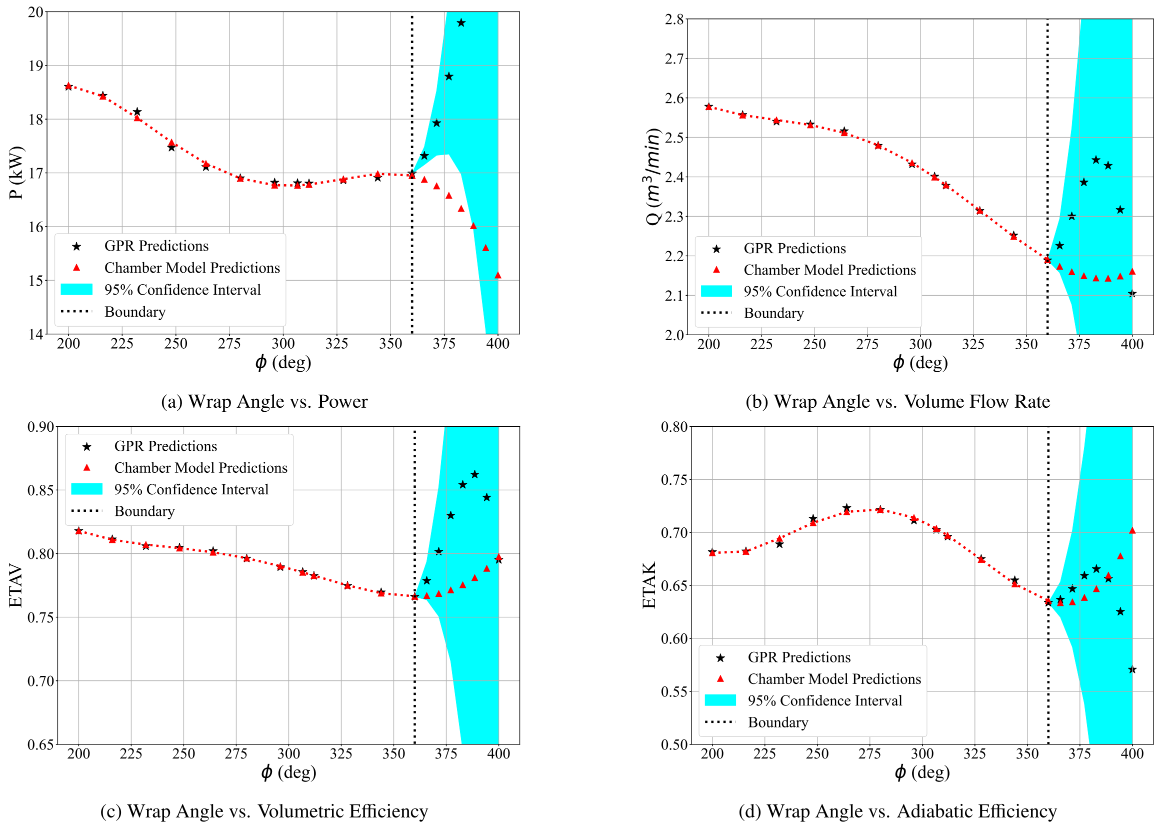
(c) Tip Speed vs. Volumetric Efficiency (d) Tip Speed vs. Adiabatic Efficiency

Fig. 7. Compressor performance predictions using the GPR model for various rotor tip speeds both in territorial and extraterritorial regions along with the uncertainties. The predictions from the physics-based chamber model are plotted together for comparison.

input parameters, which can be expensive to compute through physical experiments or simulations. Importantly, the highlight of the GPR model is to quantify the uncertainty in its predictions. To demonstrate this, the GPR model is utilized to perform predictions not only in the practical range of input parameters over which it is trained but also in the out-of-distributions, called here as extraterritorial predictions.

The GPR prediction plots for various input design parameters shown in Figs. 7, 8, 9, 10 comprises three key components, each providing valuable insights into the modeling and prediction process:

- **GPR Predictions (Black Star):** Represented by the black star markers, these data points signify the GPR model predictions for output parameters at various input values.
- **Chamber Model Predictions (Red Triangle):** The dotted red line serves as a ground truth and depicts the underlying true function that elucidates the intricate relationship between input and output parameters. This chamber model prediction acts as a benchmark for assessing the accuracy of the GPR surrogate model.
- **Uncertainty (Cyan):** The shaded cyan region enveloping the GPR predictions signifies the 95% confidence interval. This zone quantifies the uncertainty associated with the GPR model's predictions. It provides a crucial measure of the model's confidence in its estimates, allowing decision-makers to gauge the reliability of the results.
- **Boundary (Black Dotted Line):** The black dotted line denotes the training boundary of the GPR model. It separates two distinct



(a) Wrap Angle vs. Power

(b) Wrap Angle vs. Volume Flow Rate

(c) Wrap Angle vs. Volumetric Efficiency

(d) Wrap Angle vs. Adiabatic Efficiency

Fig. 8. Compressor performance predictions using the GPR model for various wrap angles both in territorial and extraterritorial regions along with the uncertainties. The predictions from the physics-based chamber model are plotted together for comparison.

Table 4
The table showcases the RMSE and R^2 values for GPR model performance on training and testing data, indicating significant improvements after hyperparameter tuning. Following optimization, the RMSE for training data improved by 92.9%, and for testing data, it improved by 94.4%. Additionally, the R^2 values showed remarkable enhancements, with an improvement of 14.4% for training data and 21.3% for testing data.

ML model	RMSE	R^2 (%)
Training result		
GPR (before tuning)	0.1532	87.3984
GPR (after tuning)	0.010889	99.9982
Testing result		
GPR (before tuning)	0.1843	82.4344
GPR (after tuning)	0.010301	99.9801

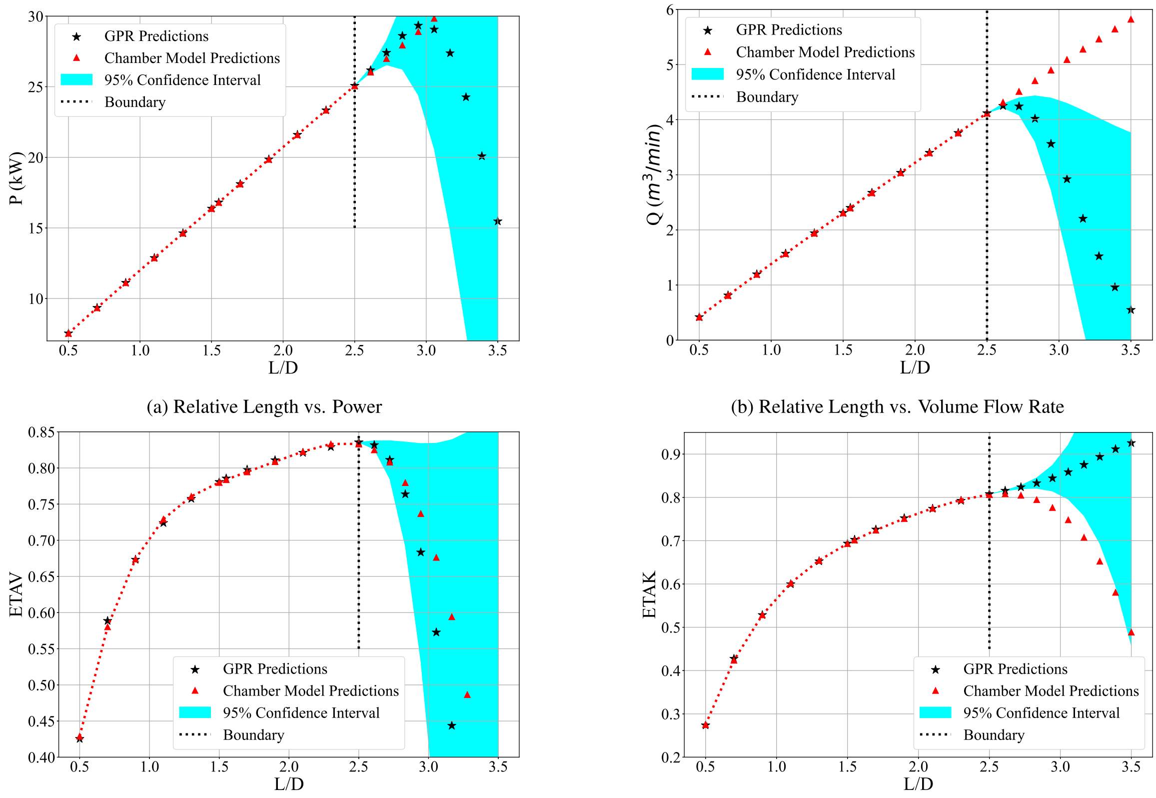
regions: the territorial region on the left, where the model has been trained using observed data, and the extra-territorial region on the right, which represents uncharted territory.

Figs. 7, 8, 9, and 10 collectively showcase the effectiveness of Gaussian Process Regression (GPR) in capturing complex relationships and estimating prediction uncertainties. It is interesting to note that the GPR model is accurate with unnoticeable uncertainties in its territorial range, while it clearly quantifies the uncertainties as the natural outcome in its extraterritorial predictions. From the results, it can be observed that the GPR model can predict the performance parameters (P, Q, ETAV, ETAK) as a function of rotor tip speed with very good accuracy not only in its territorial range but also in the extraterritorial or out-of-distribution range of the input design parameters. When it comes to the other design parameters, the GPR model performs extremely well in the territorial range but deviates from physical predictions (ground truth) in the extraterritorial range, but with quantified uncertainties. It is worth emphasizing here that, the territorial range considered in this study covers the entire practical range for compressor system design, making the GPR model suitable for prediction and optimization studies. Nonetheless, using such an uncertainty-quantified surrogate model facilitates engineers and designers to make informed decisions through its quantified prediction uncertainties.

4. Experimental validation

This section aims to verify the accuracy of the GPR based performance prediction framework within a real-world testing environment. To this end, experimental testing was conducted on the KPCL KAS-300 compressor block at the Centre for Compressor Technology, City, University of London (U.K.), employing an in-house designed air compressor test rig (Fig. 11). This test rig adheres to the stringent CAGI and PNEUROP test standards, and testing procedures are conducted in accordance with ISO 1217 guidelines.

The test compressor, driven by a variable-speed electric motor with a rating of 75 kW, reaches a rotational tip speed of up to 40 m/s through a belt drive system with a pulley ratio of 1.7. Oil injection into the compressor occurs via a main oil supply manifold, and air enters the system through the top-mounted air intake filter. Within the compressor, the air is mixed with oil and post-compression, the resulting mixture of hot oil and compressed air is discharged through a 2-inch pipe located at the compressor's base. Subsequently, this discharged mixture enters a two-stage oil separator system (Fig. 12). In the first stage, a centrifugal oil separator effectively isolates the majority of the oil from the compressed air, which is then water-cooled and reintroduced into the compressor. A minor quantity of oil in vapor form proceeds to the second-stage separator, where a filter



(a) Relative Length vs. Power

(b) Relative Length vs. Volume Flow Rate

(c) Relative Length vs. Volumetric Efficiency

(d) Relative Length vs. Adiabatic Efficiency

Fig. 9. Compressor performance predictions using the GPR model for various relative rotor lengths both in territorial and extraterritorial regions along with the uncertainties. The predictions from the physics-based chamber model are plotted together for comparison.

further extracts any remaining oil from the air. The collected oil in the second separator is not recirculated but is periodically filtered and reused. Finally, the air exits the system through a top-mounted pipeline equipped with an orifice plate for measuring the discharge flow rate. A globe valve, controlled by a stepper motor, offers precise regulation of discharge pressure and airflow rate, while a pressure relief valve, positioned atop the oil separator, serves as a safety precaution in the event of excess pressure buildup within the separator.

In this study, the performance of the KAS-300 compressor block, operating within a pressure range of 6.5 to 14.5 bar (g) and a variable speed range of 15 to 45 m/s, is investigated. The experimental analysis primarily centers on the operation of the screw compressor at a pressure ratio of 8.5. This investigation encompasses a range of tip speeds spanning from 10 to 35 m/s, while maintaining a fixed built-in volume ratio of 4.6, a relative length of 1.55, and a wrap angle of approximately 300 degrees. Throughout the experimental testing, the geometric input parameters, such as the built-in volume ratio, relative length, and rotor wrap angle, remained constant. Key performance parameters, including power consumption (P), volume flow rate (Q), volumetric efficiency ($ETAV$), and adiabatic efficiency ($ETAK$), have been measured and are shown in Fig. 13. However, owing to the proprietary nature of the industrial screw compressor's direct performance details, the presented results are normalized concerning their respective maximum values. The normalization formula is expressed as:

$$\text{Normalized Parameter} = \frac{\text{Actual Parameter} - \text{Minimum Parameter Value}}{\text{Maximum Parameter Value} - \text{Minimum Parameter Value}} \tag{5}$$

This normalization procedure facilitates the presentation of a performance map that provides insights into the operational characteristics while adhering to confidentiality constraints. Moreover, the normalization allows for meaningful comparisons and discussions without disclosing specific industrial data. For reference, Table 5 outlines the range of the output parameters considered in the experimental testing, providing a comprehensive overview of the performance metrics examined in this study.

Table 5
Range of output parameters investigated in experimental testing for the KAS-300 compressor block.

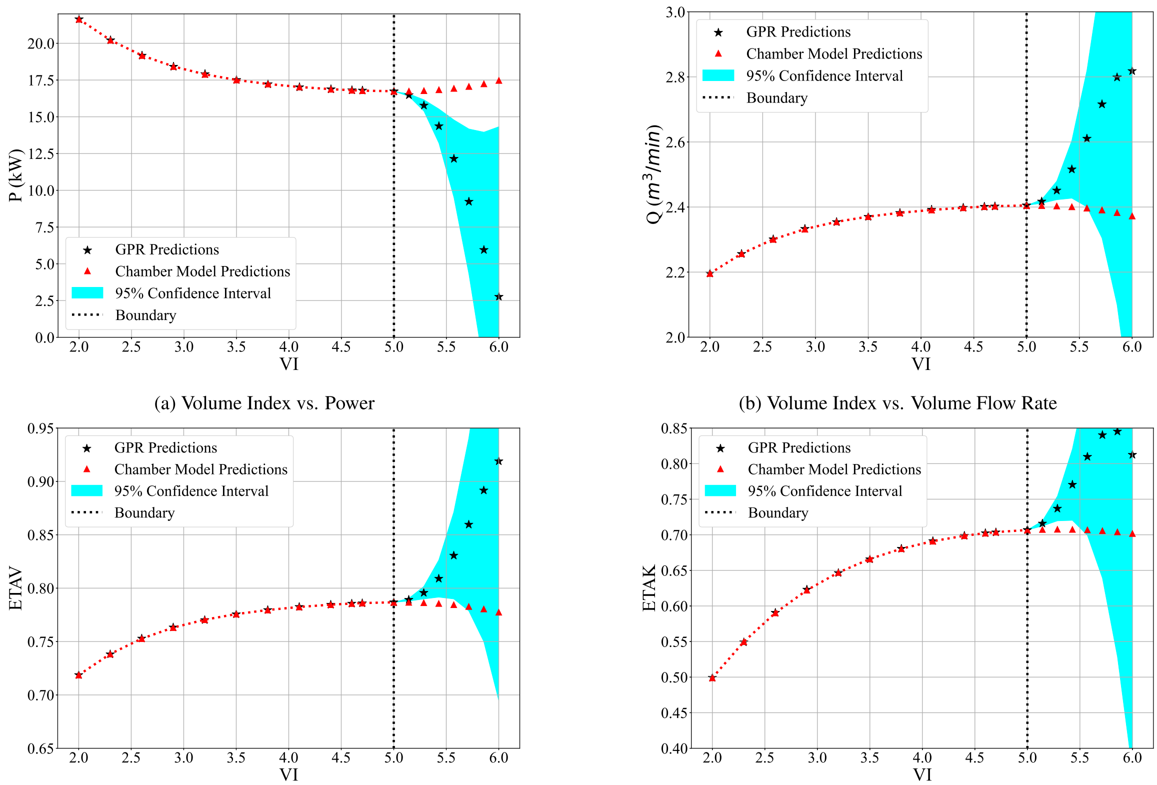
Output parameters	Range
P (kW)	(10, 60)
Q (m^3/min)	(1, 10)
ETAV (%)	(60, 100)
ETAV (%)	(70, 100)

The trained GPR model is then used to predict the performance of the above-specified compressor configuration for various tip speeds. The percentage error difference between the GPR model predictions and the experimental data is shown in Fig. 14.

$$\%\ \text{Error} = \frac{|\ \text{GPR Predictions} - \text{Experimental Data}\ |}{\text{Experimental Data}} \times 100 \tag{6}$$

The results show an overall good agreement with an acceptable deviation within the range of (+/−) 5%, validating the accuracy and reliability of the developed GPR-based performance prediction tool. The differences between the predictions and the measurements can be attributed to the testing conditions and the inherent uncertainties in the experiments.

In addition to the presented experimental results, the Gaussian Process Regression (GPR) model's performance was rigorously assessed through experimentation with diverse sets of values. The model demonstrated consistent and reliable predictions across a range of input



(a) Volume Index vs. Power
(b) Volume Index vs. Volume Flow Rate
(c) Volume Index vs. Volumetric Efficiency
(d) Volume Index vs. Adiabatic Efficiency

Fig. 10. Compressor performance predictions using the GPR model for various built-in volume ratios both in territorial and extraterritorial regions along with the uncertainties. The predictions from the physics-based chamber model are plotted together for comparison.

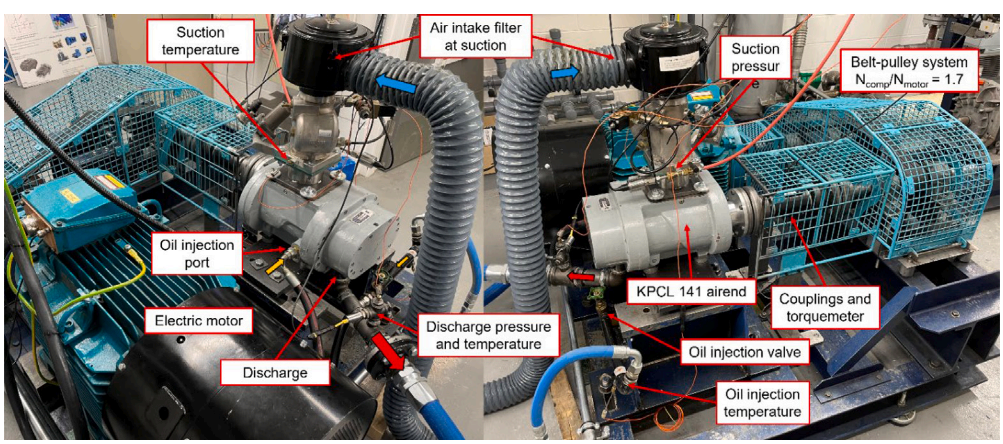


Fig. 11. Schematic labeled diagram of the compressor test rig. The diagram illustrates the complete test rig components, including the bare KAS-300 compressor, providing a comprehensive view of the experimental setup.

parameters, signifying its robustness. Sensitivity analysis further confirmed the stability of the GPR model, emphasizing its applicability in capturing the complex relationships within the dataset. These findings strengthen the credibility and versatility of the developed GPR-based performance prediction tool for screw compressors.

5. Performance optimization

In this section, the aim is to optimize the geometrical parameters of the screw compressor, specifically the wrap angle, relative length, tip speed of the male rotor, and built-in volume ratio. These parameters significantly impact the screw compressor's performance, with the objective of minimizing power consumption and maximizing the volume flow rate, volumetric and adiabatic efficiency. Bayesian optimization is chosen for its efficient search through the parameter space, leveraging the developed Gaussian Process Regression (GPR) model. The number of iterations for Bayesian optimization is set to 20.

The plot shown in Fig. 15 illustrates the process of Bayesian optimization. The y-axis represents the value of the objective function (Mean Squared Error) being minimized, while the x-axis denotes the number of iterations performed. The red marker indicates the optimal point where the objective function reaches its minimum value, highlighting the successful convergence of the optimization algorithm. Table 6 presents the input parameter range, optimal values, and optimization duration, showcasing the effectiveness of the adopted Bayesian optimization.

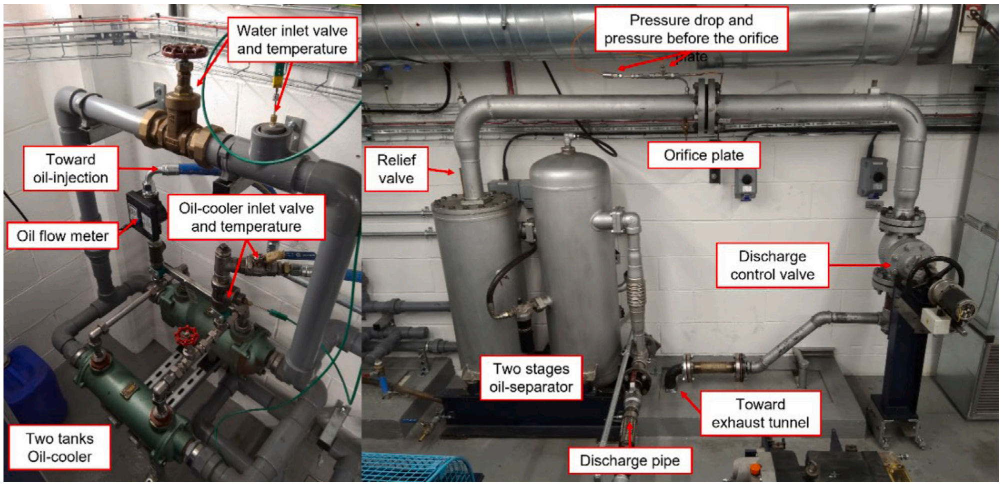
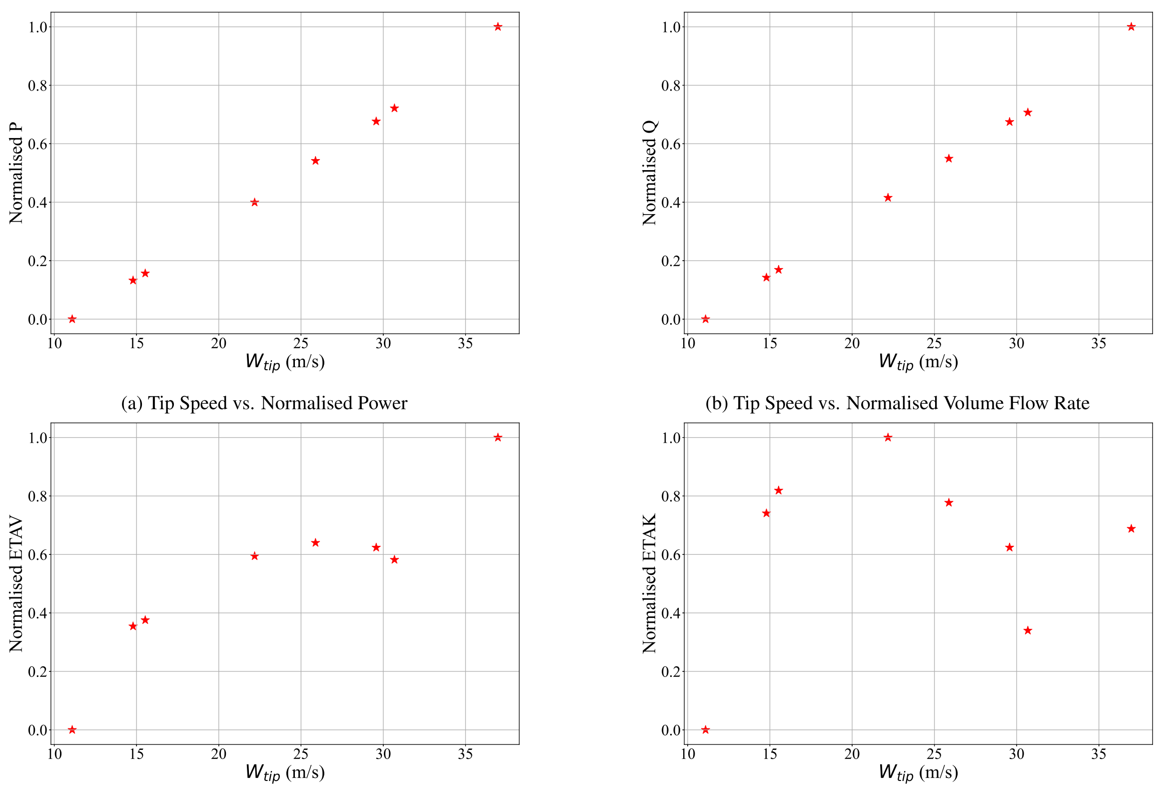


Fig. 12. Schematic representation of the compressor test rig auxiliary systems. The diagram highlights essential auxiliary connections, including control valves, oil flow meters, relief valves, etc., crucial for the comprehensive analysis of the experimental setup.



(a) Tip Speed vs. Normalised Power

(b) Tip Speed vs. Normalised Volume Flow Rate

(c) Tip Speed vs. Normalised Volumetric Efficiency (ETAV)

(d) Tip Speed vs. Normalised Adiabatic Efficiency (ETAK)

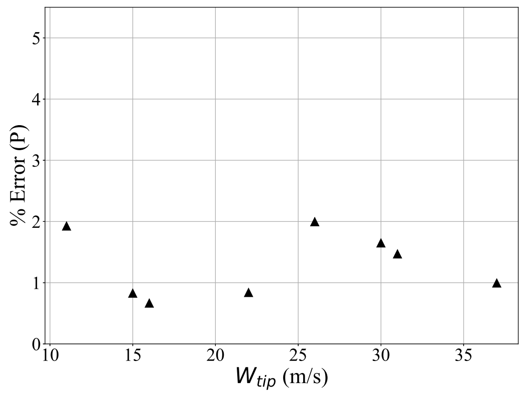
Fig. 13. Normalized experimental data showing the performance characteristics of the KAS-300 compressor block.

Table 6
Input parameters for Bayesian optimization along with the optimal values attained. The Bayesian optimization process, utilizing the GPR-based machine learning model for performance prediction, took approximately 29 min for optimization.

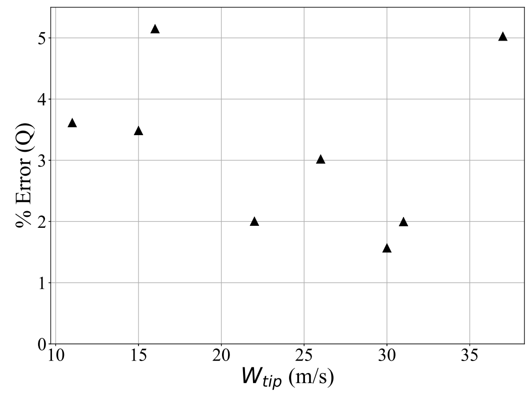
Input parameter	Range	Optimal value	Time duration (min)
W_{tip} (m/s)	(15, 45)	38	29
VI	(2, 5)	4.25	29
L/D	(0.5, 2)	2	29
ϕ (deg)	(200, 360)	335.5527	29

The achieved reduction of approximately 2% in specific power consumption for the same male rotor diameter in the oil-flooded screw compressor underscores the benefits of machine learning-based optimization.

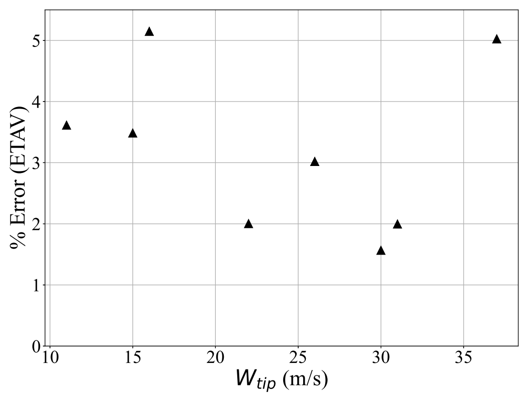
Subsequently, the optimal geometrical parameters are validated using an alternative optimization framework employing the Genetic Algorithm as the optimization algorithm and the multi-chamber model as the physics solver. The evolutionary optimization algorithm used in this study is extensively explained in Kumar et al. (2022). Results from the multi-chamber model-based evolutionary optimization shown in Table 7 align favorably with the GPR-based Bayesian optimization method, further substantiating its efficacy.



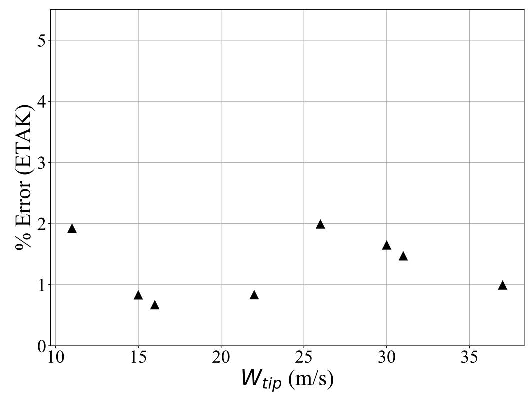
(a) Percentage error plot for power consumption



(b) Percentage error plot for volume flow rate



(c) Percentage error plot for volumetric efficiency



(d) Percentage error plot for adiabatic efficiency

Fig. 14. Percentage error difference between GPR predictions and experimental data for the compressor performance characteristics.

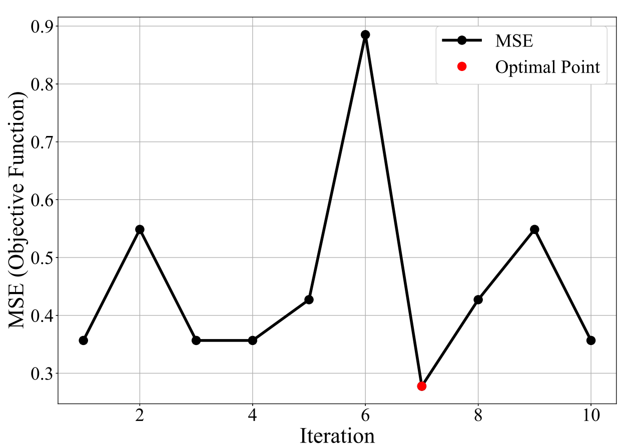


Fig. 15. Iteration process in Bayesian optimization illustrating the evolution of loss in the multi-objective function. The red dot signifies the optimal point achieved at the 7th iteration out of the 10 iterations considered for optimization.

Table 7
Input parameters for evolutionary optimization along with the optimal values attained. The optimization process, utilizing the chamber model as the solver for performance prediction and the Genetic Algorithm as the optimization method, required approximately 210 min for completion.

Input parameter	Range	Optimal value	Time duration (min)
W_{tip} (m/s)	(15, 45)	38	210
VI	(2, 5)	4.3	210
L/D	(0.5, 2)	1.99	210
ϕ (deg)	(200, 360)	330.163	210

In both optimization frameworks, the obtained optimal values remain consistent. However, it is noteworthy that the optimization variable 'L/D ratio' reaches its upper limit. This observation confirms the well-established notion that performance improves with an increase in rotor length. Nevertheless, it is essential to consider that the rotor length is restricted by the rotor bending deflection, which acts as a limiting factor rather than a variable for optimization. Introducing the allowable rotor deflection as an optimization constraint could allow us to treat the 'L/D ratio' as an optimization variable. However, in practice, the 'L/D ratio' tends to converge to the maximum deflection limit, leaving limited room for further optimization. Therefore, when determining the 'L/D ratio,' it is crucial to subject it to deflection analysis, which can serve as a constraint in the optimization framework.

6. Summary and future work

The present work successfully developed a GPR-based machine learning algorithm for predicting the performance of a screw compressor block. Utilizing Bayesian optimization for hyperparameter tuning significantly improved the model accuracy to nearly 99%. The performance prediction model was validated against experimental data, demonstrating its reliability with an acceptable deviation within the range of (+/−) 5% in real-world scenarios. Further, it was shown that utilizing GPR models in performance predictions is reliable owing to its inherent capability of quantifying the uncertainties in the predictions. The hyperparameter-tuned model was then employed to optimize screw geometrical parameters using the Bayesian algorithm, resulting in a 2% reduction in specific power consumption, which is significant in the context of compressor design. Comparison with GA-based optimization using the multi-chamber thermodynamic model demonstrated the computational efficacy of the proposed framework while providing similar optimal values.

In terms of computational feasibility, the implementation of the Gaussian Process Regression (GPR) model, including hyperparameter tuning, proved efficient and practical. The non-parametric nature of the GPR model allows it to handle complex relationships within the dataset, and the Bayesian optimization for hyperparameter tuning demonstrates computational viability with minimal iterations. Furthermore, the experimental validation conducted on the KPCL KAS-300 compressor block adhered to standardized testing procedures and employed a well-designed test rig to obtain reliable results for validation.

In future research, the aim is to enhance the generalization capabilities of the developed GPR-based machine learning algorithm. While the current study focuses on a specific screw compressor block, the importance lies in extending the model's applicability to a broader range of screw compressor sizes and configurations. Strategies including transfer learning will be explored for model development involving diverse datasets representing various compressor designs and operational settings. This expansion will contribute to a more comprehensive understanding of the algorithm's generalization potential. In turn, it facilitates the model's broader utility as an engineering tool for researchers and practitioners engaged in screw compressor design and optimization across diverse applications.

CRediT authorship contribution statement

Abhishek Kumar: Data curation, Formal analysis, Investigation, Methodology, Software, Validation, Visualization, Writing – original draft. **Sumit Patil:** Methodology, Writing – original draft. **Ahmed Kovacevic:** Methodology, Project administration, Resources, Supervision, Writing – review & editing. **Sathiskumar Anusuya Ponnusami:** Conceptualization, Methodology, Resources, Supervision, Writing – review & editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

Acknowledgments

We gratefully thank Kirloskar Pneumatic Company Limited, Pune, India for sponsoring this research. We also want to acknowledge the Centre for Compressor Technology, City, University of London for their continued guidance and support in this research.

References

Abdan, S., Stosic, N., Kovacevic, A., Smith, I., Asati, N., 2022. Oil drag loss in oil-flooded, twin-screw compressors. Proc. Inst. Mech. Eng. E J. Process Mech. Eng. 09544089221115493.

Analysis, P., 2014. SCORG - screw compressor rotor grid generation. Software Package for Design and Analysis of Positive Displacement Machines. URL: https://pdmanalysis.co.uk/scorg/.

Deng, W., Li, Z., Li, X., Chen, H., Zhao, H., 2022. Compound fault diagnosis using optimized MCKD and sparse representation for rolling bearings. IEEE Trans. Instrum. Meas. 71, 1–9.

Fontes, A., Shadmehri, F., 2023. Data-driven failure prediction of fiber-reinforced polymer composite materials. Eng. Appl. Artif. Intell. 120, 105834.

Frazier, P.I., Wang, J., 2015. Bayesian optimization for materials design. In: Information Science for Materials Discovery and Design. Springer, pp. 45–75.

Ghorbanian, K., Gholamrezaei, M., 2009. An artificial neural network approach to compressor performance prediction. Appl. Energy 86 (7–8), 1210–1221.

Gibbs, M.N., 1998. Bayesian Gaussian Processes for Regression and Classification (Ph.D. thesis). Citeseer.

Injadat, M., Salo, F., Nassif, A.B., Essex, A., Shami, A., 2018. Bayesian optimization with machine learning algorithms towards anomaly detection. In: 2018 IEEE Global Communications Conference. GLOBECOM, IEEE, pp. 1–6.

Joly, M., Sarkar, S., Mehta, D., 2019. Machine learning enabled adaptive optimization of a transonic compressor rotor with precompression. J. Turbomach. 141 (5), 051011.

Kim, T., Li, C.J., 1995. Feedforward neural networks for fault diagnosis and severity assessment of a screw compressor. Mech. Syst. Signal Process. 9 (5), 485–496.

Kopsiaftis, G., Protopapadakis, E., Voulodimos, A., Doulamis, N., Mantoglou, A., et al., 2019. Gaussian process regression tuned by bayesian optimization for seawater intrusion prediction. Comput. Intell. Neurosci. 2019.

Kovacevic, A., Rane, S., Stosic, N., 2016. Computational fluid dynamics in rotary positive displacement screw machines. In: 16th International Symposium on Transport Phenomena and Dynamics of Rotating Machinery.

Krogh, A., 2008. What are artificial neural networks? Nature Biotechnol. 26 (2), 195–197.

Kumar, A., Kovacevic, A., Ponnusami, S., Patil, S., Abdan, S., Asati, N., 2022. On performance optimisation for oil-injected screw compressors using different evolutionary algorithms. In: IOP Conference Series: Materials Science and Engineering, vol. 1267, (1), IOP Publishing, 012021.

Liu, J., Wang, X., Xie, F., Wu, S., Li, D., 2023. Condition monitoring of wind turbines with the implementation of spatio-temporal graph neural network. Eng. Appl. Artif. Intell. 121, 106000.

Ma, Y., He, Y., Wang, G., Wang, L., Zhang, J., Lee, D., 2023. Corrosion fatigue crack growth prediction of bridge suspender wires using Bayesian Gaussian process. Int. J. Fatigue 168, 107377.

MacKay, D.J., 1992. Bayesian interpolation. Neural Comput. 4 (3), 415–447.

Marx, J., Gantner, S., Städing, J., Friedrichs, J., 2018. A machine learning based approach of performance estimation for high-pressure compressor airfoils. In: Turbo Expo: Power for Land, Sea, and Air, vol. 51029, American Society of Mechanical Engineers, V02DT46A004.

Melo, J., 2012. Gaussian Processes for Regression: A Tutorial. Technical Report, University of Porto.

Morita, Y., Rezaeiravesh, S., Tabatabaei, N., Vinuesa, R., Fukagata, K., Schlatter, P., 2022. Applying Bayesian optimization with Gaussian process regression to computational fluid dynamics problems. J. Comput. Phys. 449, 110788.

Nakka, R., Harursampath, D., Ponnusami, S.A., 2023. A generalised deep learning-based surrogate model for homogenisation utilising material property encoding and physics-based bounds. Sci. Rep. 13 (1), 9079.

Nguyen, H.H., Chan, C.W., 2006. Applications of artificial intelligence for optimization of compressor scheduling. Eng. Appl. Artif. Intell. 19 (2), 113–126.

Noble, W.S., 2006. What is a support vector machine? Nature Biotechnol. 24 (12), 1565–1567.

Pathan, M., Ponnusami, S., Pathan, J., Pitisongsawat, R., Erice, B., Petrinic, N., Tagarielli, V., 2019. Predictions of the mechanical properties of unidirectional fibre composites by supervised machine learning. Sci. Rep. 9 (1), 13964.

Patil, S., Kovacevic, A., Ponnusami, S., Asati, N., 2022. Training neural networks to predict the energy efficiency of screw rotor profiles. In: Proc. 2022 Int. Compress. Eng. Conf. Purdue.

Rahbari, A., Rébillat, M., Mechbal, N., Canu, S., 2021. Unsupervised damage clustering in complex aeronautical composite structures monitored by Lamb waves: An inductive approach. Eng. Appl. Artif. Intell. 97, 104099.

Rhode, S., 2020. Non-stationary Gaussian process regression applied in validation of vehicle dynamics models. Eng. Appl. Artif. Intell. 93, 103716.

Richardson, R.R., Osborne, M.A., Howey, D.A., 2017. Gaussian process regression for forecasting battery state of health. J. Power Sources 357, 209–219.

Salcedo-Sanz, S., Rojo-Álvarez, J.L., Martínez-Ramón, M., Camps-Valls, G., 2014. Support vector machines in engineering: an overview. Wiley Interdiscip. Rev. Data Mining Knowl. Discov. 4 (3), 234–267.

Staudenmayer, J., Ruppert, D., 2004. Local polynomial regression and simulation–extrapolation. J. R. Stat. Soc. Ser. B Stat. Methodol. 66 (1), 17–30.

Sterling, D., Sterling, T., Zhang, Y., Chen, H., 2015. Welding parameter optimization based on Gaussian process regression Bayesian optimization algorithm. In: 2015 IEEE International Conference on Automation Science and Engineering. CASE, IEEE, pp. 1490–1496.

Stojanović, V., 2023. Fault-tolerant control of a hydraulic servo actuator via adaptive dynamic programming. Math. Model. Control.

Stosic, N., Hanjalic, K., 1994. Development and optimization of screw engine rotor pair on the basis of computer modeling. In: Proc. 1994 Int. Compress. Eng. Conf. Purdue, Vol. 61.

Stosic, N., Smith, I.K., Kovacevic, A., 2003. Optimisation of screw compressors. Appl. Therm. Eng. 23 (10), 1177–1195.

Stosic, N., Smith, I., Kovacevic, A., 2005. Screw Compressors: Mathematical Modelling and Performance Calculation. Springer Science & Business Media.

Taylor, J., Conduit, B., Dickens, A., Hall, C., Hillel, M., Miller, R., 2020. Predicting the operability of damaged compressors using machine learning. J. Turbomach. 142 (5), 051010.

Wang, T., Qi, Q., Zhang, W., Zhan, D., 2023a. Research on optimization of profile parameters in screw compressor based on BP neural network and genetic algorithm. Energies 16 (9), 3632.

Wang, R., Zhuang, Z., Tao, H., Paszke, W., Stojanovic, V., 2023b. Q-learning based fault estimation and fault tolerant iterative learning control for MIMO systems. ISA Trans. 142, 123–135.

Wetherill, G.B., Wetherill, G.B., 1981. Polynomial regression. Intermed. Stat. Methods 157–170.

Wuest, T., Weimer, D., Irgens, C., Thoben, K.-D., 2016. Machine learning in manufacturing: Advantages, challenges, and applications. Prod. Manuf. Res. 4 (1), 23–45.

Yadav, A., Bareth, R., Kochar, M., Pazoki, M., Sehiemy, R.A.E., 2023. Gaussian process regression-based load forecasting model. IET Gener. Transm. Distrib..

Yamashita, T., Sato, N., Kino, H., Miyake, T., Tsuda, K., Oguchi, T., 2018. Crystal structure prediction accelerated by Bayesian optimization. Phys. Rev. Mater. 2 (1), 013803.

Ying, Y., Xu, S., Li, J., Zhang, B., 2020. Compressor performance modelling method based on support vector machine nonlinear regression algorithm. R. Soc. Open Sci. 7 (1), 191596.

Zhao, H., Liu, J., Chen, H., Chen, J., Li, Y., Xu, J., Deng, W., 2023a. Intelligent diagnosis using continuous wavelet transform and Gauss convolutional deep belief network. IEEE Trans. Reliab. 72 (2), 692–702. http://dx.doi.org/10.1109/TR.2022.3180273.

Zhao, T., Song, C., Lu, S., Xu, L., 2022. Prediction of uniaxial compressive strength using fully Bayesian Gaussian process regression (fB-GPR) with model class selection. Rock Mech. Rock Eng. 55 (10), 6301–6319.

Zhao, J., Song, Y., Wang, L., Guo, H., Marigentti, F., Liu, X., 2023b. Forecasting the eddy current loss of a large turbo generator using hybrid ensemble Gaussian process regression. Eng. Appl. Artif. Intell. 121, 106022.

Ziviani, D., Bell, I.H., Zhang, X., Lemort, V., De Paepe, M., Braun, J.E., Groll, E.A., 2020. PDSim: Demonstrating the capabilities of an open-source simulation framework for positive displacement compressors and expanders. Int. J. Refrig. 110, 323–339.