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Research paper

Domain-informed operation excellence of gas turbine system with machine learning

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ABSTRACT

The domain-consistent adoption of artificial intelligence (AI) remains low in thermal power plants due to the black-box nature of AI algorithms and low representation of domain knowledge in conventional data-centric analytics. In this paper, we develop a MAhalanobis Distance-based OPTimization (MAD-OPT) framework that incorporates the AI models and Mahalanobis distance-based constraint to introduce domain knowledge into data-centric analytics. The developed MAD-OPT framework is applied to maximize thermal efficiency and minimize turbine heat rate for an industrial 395 MW capacity gas turbine system. Artificial neural network (ANN) models are trained to predict thermal efficiency, power and turbine heat rate with more than 95% accuracy on the test dataset. The MAD-OPT framework yields 0.1 percentage point relative improvement in thermal efficiency during complete power ramp-up from gas turbine system when operated at ambient temperature of 22 °C than at 34 °C. The robust-optimal values of thermal efficiency (40.99 ± 0.16%) and turbine heat rate (8820 ± 32.82 kJ/kWh) are estimated at the power generation of 305 MW and ambient temperature of 26 °C. More importantly, the framework is successfully deployed to estimate optimal process conditions beyond the design limit of the gas turbine system, addressing the barrier of ANN-based extrapolation in untrained operating space. We also demonstrate that implementing data-centric optimization analytics without incorporating domain-informed constraints may provide ineffective solutions that may not be implementable in the real operation of the gas turbine system. The MAD-OPT framework has demonstrated to adapt with the real-time operating constraints of industrial operations of gas turbine system which may advance the safe and domain-compliant AI adoption to enhance the operation excellence of thermal power systems.

1. Introduction

Combined cycle gas power plants are crucial to allow for the shift of the energy mix from high to low emissions, especially in energy systems dominated by thermal plants [1,2]. Combined cycle gas power plants can rapidly increase their power output for peak energy demand, produce lower CO_2 emissions, and generally have higher energy efficiency than coal power plants [3]. Therefore, effective monitoring of gas power plant performance metrics, including thermal efficiency and turbine heat rate, is critical to maintaining an economic mode of operation that is complemented by a lower emissions discharge to the environment. Furthermore, accurate modeling and optimization of performance metrics for gas turbine systems is a fundamental task for effective operation of gas power plants that improves operational excellence and supports the achievement of the net zero target from the energy sector [4].

In recent years, artificial intelligence (AI) and machine learning (ML) models have demonstrated good performance in the modeling of complex systems due to their ability and capacity to learn from sparse as well as big data [5–12]. With reference to power systems and particularly to gas power plants, AI models, including artificial neural network (ANN), support vector machine, and ensemble methods, are deployed to model or forecast electric power generation and emissions discharge from combined cycle gas power plants [13–15]. These studies

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Nomenclature

Symbol/Acronym	Description
AH	Ambient Humidity (%)
AP	Ambient Pressure (hPa)
AT	Ambient Temperature (°F)
AI	Artificial Intelligence
ANN	Artificial Neural Network
R^2	Coefficient of Determination
CDP	Compressor Discharge Pressure (psi)
CDT	Compressor Discharge Temperature (°F)
FGEXT	Flue Gas Temperature at HRSG Inlet (°C)
FGT	Fuel Gas Temperature (°F)
GFFR	Gas Fuel Flow Rate (lb/s)
GT	Gas Turbine
MAD-OPT	MAhalanobis Distance-based OPTimization
ML	Machine Learning
PCC	Pearson Correlation Coefficient
PHGOT	Performance Heater Gas Outlet Temperature (°F)
Power	Power Generation (MW)
RMSE	Root Mean Square Error
$Power_{\text{Set Point}}$	Set Point of Power Generation
SHAP	Shapley Additive Explanations
TE	Thermal Efficiency (%)
THR	Turbine Heat Rate (kJ/kWh)

are mainly based on open source data sets related to gas power plants available in the UC Irvine machine learning repository [16,17].

Despite the excellent potential of AI to model complex functions, its adoption in real-time operation control and management for gas power plants remains marginally low [4]. The low adoption rate of AI in the safety critical operation of gas power plants stems from the inaccessibility of high-resolution industrial datasets of combined-cycle gas power plants, the black-box nature of most AI algorithms, the low explainability of model predictions, and insufficient representation of domain knowledge in data-centric analytics. A key barrier to AI adoption in industrial operations is the lack of domain consistency in the results produced by AI-based optimization routines. When AI models are integrated into optimization frameworks without incorporating explicit domain-informed constraints, the estimated optimized conditions may violate the operating restrictions or physical laws [18]. The disconnect of domain knowledge in the formulation of optimization problems undermines trust and limits the practical deployment of AI-based solutions in high-stakes industrial environments [19].

Literature review is conducted to identify the state-of-the-art in applying AI/ML for modeling and optimization of the performance of the gas power plants. Zhang et al. [20] and Xezonakis et al. [21] have investigated the efficacy of different AI-based modeling algorithms to predict the power generation from gas power plants. Osegi et al. [22] developed an evolutionary programming and continual learning neural network approach to predict the power output from an open-cycle gas power plant. The effect of ambient temperature on the power generation from the gas turbine system was also investigated. Wu et al. [23] trained ML models to predict CO-NO_x emissions from a natural gas power plant. The proposed methodology built on the feature optimization scheme improved the predictive performance of the ML model by 18%– 67 %. In another study, Manatura et al. [24] utilized process variables and ambient conditions to train an ANN model for predicting the turbine heat rate of a gas turbine system.

Researchers have also implemented empirical and fuzzy logic-based constraints for the power generation operation of gas power plants. Mamlook et al. [25] and Bertini et al. [26] have implemented fuzzy rule-based domain knowledge of the gas turbine system for guiding the optimization solvers to avoid unsafe and inefficient operating conditions for the gas power plant. PI/PD controller [27] as well as model predictive control schemes are also applied to improve the operation and efficiency of the power generation of the gas power plant [28–30]. Moreover, deterministic and evolutionary optimization techniques, embedding the neural networks in the optimization problems, are also implemented for performance analysis of gas power plants [31–33].

The literature studies have reported the effectiveness of AI models, fuzzy logic, model predictive control, optimization techniques and empiric bounds on the process variables for the control of gas power plant. However, several issues remain unexplored, (i) the constraints can be univariate, require rule-based manual tuning, and can neglect the multivariate interaction that is a typical operating characteristic of the gas power plant's operation, (ii) the domain-consistency of the optimal solutions with the operating characteristics of the gas power plant remains largely unexplored for gas power plant which is a critical consideration for their implementation on the operation of gas power plant, (iii) The robustness evaluation of the ML model-based predictions is important for industrial applications considering the evolving process conditions and uncertainty in the measurements [34,35]. However, the robustness evaluation of AI-driven optimal solutions for the operation of gas turbine system is rarely investigated. (iv) Finally, the extrapolation of trained ML models beyond the training space, where the model-based predictions are highly uncertain [36], making them unsuitable for estimating the effective process conditions to produce power beyond the design capacity of gas turbine system. This research challenge is critical for the application of AI models in industrial systems where the process conditions evolve quickly and AI models may need to extrapolate beyond their training space to meet the industrial requirements. The identified research gaps are the key barriers in accelerating the scalable, safe and trust-worthy AI adoption rate in safety critical industrial operations and addressing them may unlock the potential of AI for the operation excellence of gas power plants [4].

This research paper presents MAhalanobis Distance-based OPTimization (MAD-OPT) framework that integrates the data-driven domain of gas turbine system in the optimization problem - a novel approach for estimating the domain-consistent optimal solutions to address the gaps identified from literature. Embedding the variable's dependency structure through the Mahalanobis distance as a constraint in the optimization problem overcomes the issues with manually tuned fuzzy rules and streamlines the representation of domain knowledge into the optimization routines. The Mahalanobis distance-based constraint constructs a multivariate ellipsoid that dynamically updates the internal correlation structures of the process variables, satisfies the multivariate interaction and dependencies among the variables in the optimization routine. This enables MAD-OPT framework to provide domain-compliant robust optimal solutions and reduce the risks of operational infeasibility of the estimated solutions for industrial applications. This is the key novelty of this research that overcomes the potential issue of implementation of the AI-based optimal results in industrial environments due to their domain-inconsistency. Moreover, the MAD-OPT provides a domain-consistent approach to estimate the robust process conditions for producing power beyond the design limit of gas turbine system – a novel solution in extrapolating AI models in untrained operating space.

The key contributions of this research paper are as follows:

- The MAD-OPT framework is empirically validated on an industrial 395 MW gas turbine system, demonstrating its capability to optimize thermal efficiency and turbine heat rate across the entire power ramp-up operating regime,
- The MAD-OPT framework has demonstrated domain-consistent extrapolation of AI models and has estimated the process conditions to produce power beyond the design capacity of the gas turbine system,

- A critical comparison reveals that omitting the Mahalanobis constraint from the optimization problem results in estimating the domain-inconsistent solutions, underscoring its necessity for preserving variable dependency structures in the estimated optimal solutions and their implementation on the gas turbine system,
- The robustness of optimized solutions is rigorously evaluated via Monte Carlo simulations, while the broader implications for operational excellence and AI integration in gas power plant management are discussed, highlighting the capability of the MAD-OPT framework to adapt with the industrial environment, and
- It is anticipated that the MAD-OPT framework may accelerate the AI-adoption rate in safety-critical industrial applications like power generation from gas turbine system since it provides domain-consistent and uncertainty-aware optimal solutions which are effective and implementable on the real-time operation of industrial systems.

The rest of the paper is organized as follows: Section 2 describes the key stages included in the MAD-OPT framework. Results and the associated discussions related to ANN model development, data-centric optimization of gas turbine system, ramping up gas turbine system under different ambient conditions, robustness evaluation of optimal solutions, operating the gas turbine system beyond the capacity discharge limit and the subsequent robustness evaluation are presented in Section 3. Later, conclusions, limitations and future work are explained in the paper.

2. Data and methods

2.1. Data acquisition

The MAD-OPT framework is applied for data-centric operation excellence analysis of a 395 MW capacity gas turbine system. A brief description of the power generation operation of the gas turbine system is provided.

The airflow rate is maintained by the air compressor while the natural gas compressor passes the natural gas through the heaters to raise its temperature, and natural gas is injected into the combustion chamber. The hot flue gases are produced in the combustion chamber from the combustion of natural gas and are passed through the gas turbine, where they expand and drive the rotor of the generator for producing electrical power. The exhaust of the flue gases from the gas turbines is made to pass through a heat recovery steam generator (HRSG) in the combined cycle gas power plant where heat is recovered from the exhaust flue gases and a steam cycle is in operation for power production. The combined cycle gas power plants typically have higher energy efficiency than the open-cycle gas power plaplants,ere exhaust flue gases are discharged to the environment. We have conducted a literature review [37–40] and have also taken feedback from process and performance engineers to identify the operationally relevant input variables of the process. We identify the relevant process input variables and the associated dataset from [41] in line with the suggestions of the plant's performance and process engineers. We have also augmented the data with another process variable, namely "Flue Gas Temperature at HRSG Inlet" to further enrich the dataset. The compiled dataset is utilized to model the performance variables of the gas turbine system, including power (MW), thermal efficiency (%) and turbine heat rate (kJ/kWh). Thermal efficiency is a ratio of electrical energy produced from the chemical energy of the gas. The turbine heat rate measures the amount of thermal energy required to produce one unit of electricity. The two performance variables have a direct link with the cost of operation of the power generation and are critically controlled to maintain efficient power generation and reduce emissions discharge from the power plant.

During the power generation operation from the gas power plant, the process variables have very different operating ranges. A significant deviation between the operating scales of the process variables negatively affects the functional mapping between the input–output variables that are constructed in the data-driven or AI models. To address this issue, we have scaled the data associated with the process variables and the performance variables on the scale of [0,1] using the following equation:

$$X_i^{\text{scaled}} = \frac{X_i - (X_i)_{min}}{(X_i)_{max} - (X_i)_{min}} \tag{1}$$

here, X_i^{scaled} is the variable that is transformed on a scale [0,1], and $(X_i)_{min}$ and $(X_i)_{max}$ represent the minimum and maximum values of the input variables, X_i, respectively. The operation of a gas power plant undergoes a smooth transition when power is increased or decreased. It is natural to have collinear process variables which are monitored during the power generation operation of a gas turbine system. A pairwise collinearity measurement allows exploration of the dependencies of the variables in a structured way, and all possible combinations of bivariate collinearity can be investigated. Pearson's correlation coefficient (PCC) measures the linear dependencies between the pair of variables, and correlation couplings between the process variables can be visualized using a heat map. The mathematical expression of PCC is given as:

$$PCC_{xy} = \frac{\sum_{i=1}^{N}(x_i - \bar{x}_i)(y_i - \bar{y}_i)}{\sqrt{\sum_{i=1}^{N}(x_i - \bar{x}_i)^2 \sum_{i=1}^{N}(y_i - \bar{y}_i)^2}} \tag{2}$$

here, $x_i \& y_i$ is a variable pair that has observations, $i = 1, 2, 3, \dots, N$. $\bar{x}_i$ and $\bar{y}_i$ are calculated as the mean of x_i and y_i, respectively. A value of PCC that reaches +1 is an indicator of strong positive correlation and vice versa. Thus, the nature of the correlation (positive or negative) can be identified by PCC. It is important to mention here that the calculated PCC is not just an indication of the correlation structures that exist in the data set. Rather, the carefully chosen process-related variables provide the rationale for treating these correlation values as relevant information regarding the operating characteristics of the system. Thus, PCC or relevant statistical metrics compute the data-centric quantification of domain knowledge present in the raw measured data. The quantification of data-driven domain knowledge as a statistical metric serves as a ground truth to evaluate the efficacy of data-driven optimization solutions, as explained in the results section.

2.2. ANN model development and feature importance analysis

ANN is a universal function approximator [42] and can find nonlinear and hidden variable structures in data [43–46]. A key advantage of using the ANN model is the computational overhead memory requirements, which are reasonable to model the complex function space on ill-defined problems [47]. A three-layer shallow ANN structure has been found useful for modeling various types of problems [48,49], and it has been proved in the literature that a shallow ANN model can approximate any nonlinear function with arbitrary accuracy given that a sufficient number of neurons are embedded in the hidden layer [50]. The information flow and processing occurring in the computational layers of ANN are mathematically represented in the following:

$$\hat{y} = f_2\left(\sum W_2.f_1\left(\sum W_1.X^T + b_1\right) + b_2\right) \tag{3}$$

here, W_1 and W_2 are the weight matrices from input-hidden and hidden-output layer of ANN model, respectively. b_1 and b_2 are the bias parameters as well as f_1 and f_2 are the activation functions implemented at the hidden and output layers of the ANN model, respectively. X^T is a set of input variables, having finite data associated with the variables which are processed at the hidden and output layer of ANN model through Eq. (3)). Resultantly, a trained ANN model simulates a response ($\hat{y}$) against the input conditions of X.

Before tuning of model parameters, the structure of shallow ANN model needs to be initialized. Rectified Linear unit (ReLu) activation function is implemented on the hidden layer of ANN model since it hedges against the vanishing gradient problem and promotes faster and efficient training of model, which is also suitable for extrapolation of ANN model [51]. Whereas, linear activation function is applied on the output layer of ANN to streamline the simulation from the ANN model. L_1 regularization is implemented to promote generalize performance of the trained model; whereas the hyperparameter (λ_1) is optimized. Initially, the hyperparameters, including number of neurons in the hidden layer, learning rate, λ_1 and λ_2 (weight decay) for Adaptive Moment Estimation (ADAM) optimizer are optimized by Tree Parzen Estimator solver [52]. Later, the optimized hyperparameters are embedded in the architecture of ANN model for tuning the parameters (W_1, W_2, b_1 and b_2). For this task, a loss function is customized that includes mean square error and L_1 regularization terms as represented in the following:

$$L = \frac{\sum_{i=1}^{N}(y_i - \hat{y}_i)^2}{N} + \lambda_1.\Theta \tag{4}$$

The back-propagation of error is the working mechanism for tuning the parameters of ANN [47], that contributes to the training of the model. The optimization solver, ADAM, is implemented that has stable and efficient performance for the training of ANN model [53]. A data split ratio of 0.8 and 0.2 is used for data partitioning into training and testing datasets, respectively. The model training is stopped either on exploitation of iterative budget or patience count in the successive improvement in the loss is crossed. The training of ANN models is implemented using PyTorch in Python.

The trained ANN models are evaluated by the coefficient of determination (R^2) and the root mean squared error (RMSE) [54] which are computed as:

$$R^2 = 1 - \frac{\sum_{i=1}^{N}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{N}(y_i - \bar{y}_i)^2} \tag{5}$$

$$RMSE = \sqrt{\frac{\sum_{i=1}^{N}(y_i - \bar{y}_i)^2}{N}} \tag{6}$$

Here, y_i, $\hat{y}_i$ are the actual and model-based simulated responses, respectively; while, $\bar{y}_i$ is calculated as the mean of y_i. R^2 varies between 0 to 1 and is considered as accuracy measure. Whereas, RMSE computes the mean error induced in the point-prediction made by the trained model. The smaller the RMSE, a better and well-trained model is developed and vice versa. These two metrics are frequently deployed to evaluate the predictive accuracy of the trained models for tabular datasets in different applications [55,56], and thus, are implemented in this paper for the evaluation of ANN models trained to predict performance variables of gas turbine system.

The feature importance analysis is performed using the Shapley Additive Explanations (SHAP) method. SHAP values are calculated using a game theory technique and compute the marginalized contribution of each feature of the model to the predictions [57]. SHAP is found to be useful in explaining the predictions made by AI models in various studies [45,58] and is applied to establish the importance of the feature in predicting performance variables (power, thermal efficiency, and turbine heat rate) of the gas turbine system.

2.3. Mahalanobis distance as a domain-informed constraint

The Mahalanobis distance is a multivariate distance metric that measures how far a point lies from the mean of the distribution, following the correlation structure in the data [59]. The Mahalanobis distance can be computed on a multivariate vector. Mathematically, the Mahalanobis distance is written as:

$$d_M(\mathbf{x}) = \sqrt{(\mathbf{x} - \boldsymbol{\mu})^\top \Sigma^{-1}(\mathbf{x} - \boldsymbol{\mu})} \tag{7}$$

here, $\mathbf{x}$ is a vector of variables that is made mean-centered through $(\mathbf{x} - \boldsymbol{\mu})$. Σ is a covariance matrix and encodes how the variables vary together. The diagonal terms are the variances of the variables, while off-diagonal terms represent the correlations between the variables. Taking the inverse of Σ scales the variables in each direction and removes the correlation between the variables. The mathematical operations compute the Mahalanobis distance ($d_M(\mathbf{x})$) and the large value of $d_M(\mathbf{x})$ means that the point is far from the mean μ and vice versa.

It is important to note here that the highly correlated variables do not contribute much to the computation of $d_M(\mathbf{x})$ than the orthogonal change (less correlated variables). This preserves the elliptical shape of the data cloud, where a large variance along the ellipse is the highly correlated direction. Thus, the Mahalanobis distance makes an ellipsoid around the multivariate data distribution and is used for outlier detection [60] or classification tasks [61] when the observed point does not fall within the ellipsoid. $d_M(\mathbf{x})$ can be set as a constraint since the calculated distance indicates how many standard deviations the point is from the mean. For example, $d_M(\mathbf{x}) = 1$ means that the point $\mathbf{x}$ is one standard deviation away from $\boldsymbol{\mu}$. Algebraically, an ellipsoid is defined in the p-dimensional space, and the region of the ellipsoid is controlled by τ as expressed in the following equation.

$$(\mathbf{x} - \mu)^\top \Sigma^{-1}(\mathbf{x} - \mu) \le \tau^2 \tag{8}$$

Geometrically, the contour $d_M(\mathbf{x}) = \tau$ is an ellipsoid centered on μ whose axes align with the principal components of Σ. Since τ adjusts the region of the ellipsoid, it is a natural setting to introduce the Mahalanobis distance as a constraint in the optimization problems for two reasons: (i) the Mahalanobis distance handles the multivariate dependencies and preserves the correlation structures. This is aligned with the operation characteristics of the gas power plant in which we have correlated variable dependencies, and we want to represent them in an optimization problem for estimating domain-informed solutions, and (ii) we can adjust the ellipsoid region and may extrapolate the design space of the power plant. For example, if a gas power plant has a designed power generation capacity of 380 MW, we may use multivariate information and τ to estimate the new process conditions to produce power beyond 380 MW.

2.4. Formulation of optimization problem and robustness evaluation of the optimal solutions

Thermal efficiency and turbine heat rate are the two critical performance variables measured in the sustained state of power generation from the gas turbine system. The objective of the optimization problem is to maximize thermal efficiency and minimize turbine heat rate at the set value of power. Since thermal efficiency and turbine heat rate exhibit nonlinear operating characteristics with process variables, the optimization problem is formulated with a nonlinear programming framework. The optimization problem embeds the trained ANN models for power, thermal efficiency, and turbine heat rate. Moreover, the Mahalanobis distance-based constraint is also incorporated in the optimization problem which is written in the following.

Objective function:

$$\min_{\mathbf{x}} f(\mathbf{x}) = -f_{\mathrm{TE}}(\mathbf{x}) + f_{\mathrm{THR}}(\mathbf{x})$$

Subject to

$$h(\mathbf{x}) = 0$$

$$(f_{\mathrm{Power}}(\mathbf{x}) - Power_{\text{ Set Point}})^2 < \epsilon$$

$$(\mathbf{x} - \mu)^\top \Sigma^{-1}(\mathbf{x} - \mu) \le \tau^2$$

$$\mathbf{x} = \{x_1, x_2, \dots, x_m\} \tag{9}$$

$$\mathbf{x} \in \mathbf{X} \subseteq \mathbf{R}^n$$

$$\mathbf{x}^L \le \mathbf{x} \le \mathbf{x}^U$$

here, $h(\mathbf{x})$ is the equality constraint, representing trained ANN models for power, thermal efficiency, and turbine heat rate. The trained ANN model predicts the responses on the scale of [0,1], so scaling is not performed for the terms included in the objective function. $Power_{\text{Set Point}}$ is set by the user from the operating space of the gas turbine operation so that its square difference from f_{Power} is minimized to ϵ. The Mahalanobis distance-based constraint is also incorporated into the optimization problem to satisfy the variable dependencies while estimating an optimal solution for the objective function. $\mathbf{x}$ is a set of operating variables, $x_1, x_2, \ldots, x_m$ that are continuous and serve as the dimensions of the search space. The lower bounds ($\mathbf{x}^L$) and the upper bounds ($\mathbf{x}^U$) are set in $\mathbf{x}$ to limit the search space for the solver and estimate a solution within the operating bounds.

The optimization problem is analyzed by two approaches: (1) the MAD-OPT framework and (2) when we did not embed the Mahalanobis constraint into the optimization problem. The two optimization problems are implemented in Pyomo and are solved by the Sparse Nonlinear OPTimizer (SNOPT) solver [62] through GAMS. The same initial guesses are used to solve the two optimization problems, and then a systematic comparison is made to analyze the implementability of the estimated solution in the gas turbine system.

The robustness of the estimated optimal solutions of the three performance variables is evaluated under perturbed process conditions. 1000 Gaussian noise observations are generated on 1% of the standard deviation of process variables and are added with the optimal process input conditions. This procedure is repeated for 50 rounds of Monte Carlo simulations to fully explore the effect of noise generation and its impact on the variability of the optimal values of the turbine heat rate and thermal efficiency with respect to the set power value. A 95% confidence interval is calculated (97.5th quantile - 2.5th quantile) for each round of Monte Carlo simulations to account for variation in the performance variables. A robust solution has a narrow confidence interval when evaluated on the perturbed process variables and vice versa.

2.5. Extrapolating the ANN model

The Mahalanobis distance measures the multivariate dependencies and handles the correlations that exist in the data. We have developed the Mahalanobis-based constraint in the optimization problem as an extrapolation framework to extrapolate the ANN. This is because when the optimization solver estimates the optimal process conditions in the extrapolated zone of ANN, the Mahalanobis distance-based constraint guides the solver to comply with variable dependencies and interactions that are established amongst the process variables. For this investigation, we took a subsample space from the actual data of the gas power plant, that is, actual gas turbine system data have power generation up to 395 MW and we separate the actual data up to 380 MW. The remaining data set, having power ranging from 381 MW to 395 MW, is separated to serve as the ground truth during extrapolation analysis. The subsample space is deployed to train the ANN models, which can predict power with reasonable accuracy up to 380 MW since the subsample space was exposed to the ANN models during the training and testing phases. Later, the extrapolation analysis is carried out on the set values of power of 385 MW, 390 MW, and 395 MW.

2.6. Verification of the MAD-OPT framework

The proposed MAD-OPT framework is applied for estimating the optimal process conditions during the power ramp-up and capacity enhancement of a 395 MW capacity gas turbine system. Contour plots are made of the process variables, and ellipses are drawn around the data distribution, which establish the feasible operating regions for the power plant's operation. The estimated optimal solutions are mapped on the contour plots in order to verify the efficacy of the optimal solutions for their implementability in the plant's operation. Moreover, the extrapolated solutions are also compared with the actual data of the power plant to verify their effectiveness and, in turn, the ability of the MAD-OPT framework for the power generation capacity enhancement of the gas turbine system.

3. Results & discussions

3.1. Gas turbine system operation

Gas turbine systems are installed to meet the peak energy demand of the grid. Although gas power systems maintain power generation capacity discharge into the grid, thermal efficiency and turbine heat rate are the key performance metrics that affect the cost of operation of the gas turbine system. The two performance metrics are driven by the operating levels of the process variables. In this paper, we analyze three performance variables, namely, the generation of power from a gas turbine system (Power - MW), thermal efficiency (TE -%) and turbine heat rate (THR - kJ/kWh) of an industrial gas turbine system of 395 MW capacity. The input variables of the process taken in this paper to analyze three performance variables of the gas turbine system are: Compressor Discharge Pressure (CDP - Psi), Gas Fuel Flow Rate (GFFR - lb/s), Fuel Gas Temperature at the inlet of the combustion chamber (FGT - °F), Ambient Temperature (°C), Ambient Pressure (AP - hPa), Ambient Humidity (AH -%), Performance Heater Gas Outlet Temperature (PHGOT - °F), Compressor Discharge Temperature (CDT - °F), and Flue Gas Temperature at HRSG inlet (FGEXT - °C). These variables affect the operating characteristics of gas turbine system and are adjusted to maintain the power generation at the desirable level. The descriptive statistics of the collected dataset like minimum, median, maximum and standard deviation (std), are computed and are mentioned in Table 1. The dataset covers wide operating range in the power generation, i.e., from 185 MW to 395 MW from gas turbine system. A noticeable variation in thermal efficiency (32.69% to 42.97%, std: 2.36) and turbine heat rate (8377 kJ/kWh to 11022 kJ/kWh, std: 579.46) is observed, highlighting the potential of data-mining and room of improvement in the energy efficiency gains through AI-led optimization analytics.

The kernel density estimate (KDE) curves are plotted separately for ambient conditions (AT, AP, and AH) and process input variables (CDP, GFFR, FGT, PHGOT, CDT, and FGEXT) as shown in Fig. 1(a). The data density curves of the ambient conditions appear to be different from each other. However, process input variables seem to have nearly similar KDE curves except PHGOT. This is further confirmed with a heat map based on Pearson's correlation coefficients, made on the pairs of process input-input and input–output variables, and are represented on Fig. 1(b). This demonstrates that process input variables have multivariate dependencies and correlation structures that characterize the power generation dynamics of the gas turbine system. In addition, the three performance variables are also correlated, depicting the operating behavior of the gas turbine system. To further explore the dependencies amongst the three performance variables (Power, TE and THR), a function space is constructed which is found to be non-convex and depicts non-linear curvature. Similarly, multivariate dependencies of varying degrees of correlation are observed with the three performance variables of the gas turbine system. This highlights the need to carry out robust data-driven analytics, which remain domain-consistent and compliant with the operating characteristics, for enhancing the AI-powered operation excellence of the gas turbine system.

3.2. Data-driven modeling of the performance variables of the gas turbine system

Fig. 2(a) shows the modeling performance of ANN models trained to predict the thermal efficiency (%), power (MW) and turbine heat rate (kJ/kWh) of gas turbine system. The trained ANN model for predicting thermal efficiency has 16 neurons in the hidden layer. The model

Table 1
Descriptive statistics of variables of gas turbine system.

Variable	Unit	Minimum	Median	Maximum	Standard Deviation
Compressor Discharge Pressure (CDP)	Psi	186	232	312	36.82
Gas Fuel Flow Rate (GFFR)	lb/s	29	38	50	5.65
Fuel Gas Temperature (FGT)	°F	484	518	535	14.93
Ambient Temperature (AT)	°C	20	26	34	3.67
Ambient Pressure (AP)	hPa	983	989	992	1.99
Ambient Humidity (AH)	%	34	68	98	14.16
Performance Heater Gas Outlet Temperature (PHGOT)	°F	400	411	425	2.47
Compressor Discharge Temperature (CDT)	°F	813	848	926	34.26
Flue Gas Temperature at HRSG Inlet (FGEXT)	°C	629	6569	673	15.90
Thermal Efficiency (TE)	%	32.69	39.02	42.97	2.36
Power Generation (Power)	MW	185	280	395	59.32
Turbine Heat Rate (THR)	kJ/kWh	8377	9225	11 022	579.46

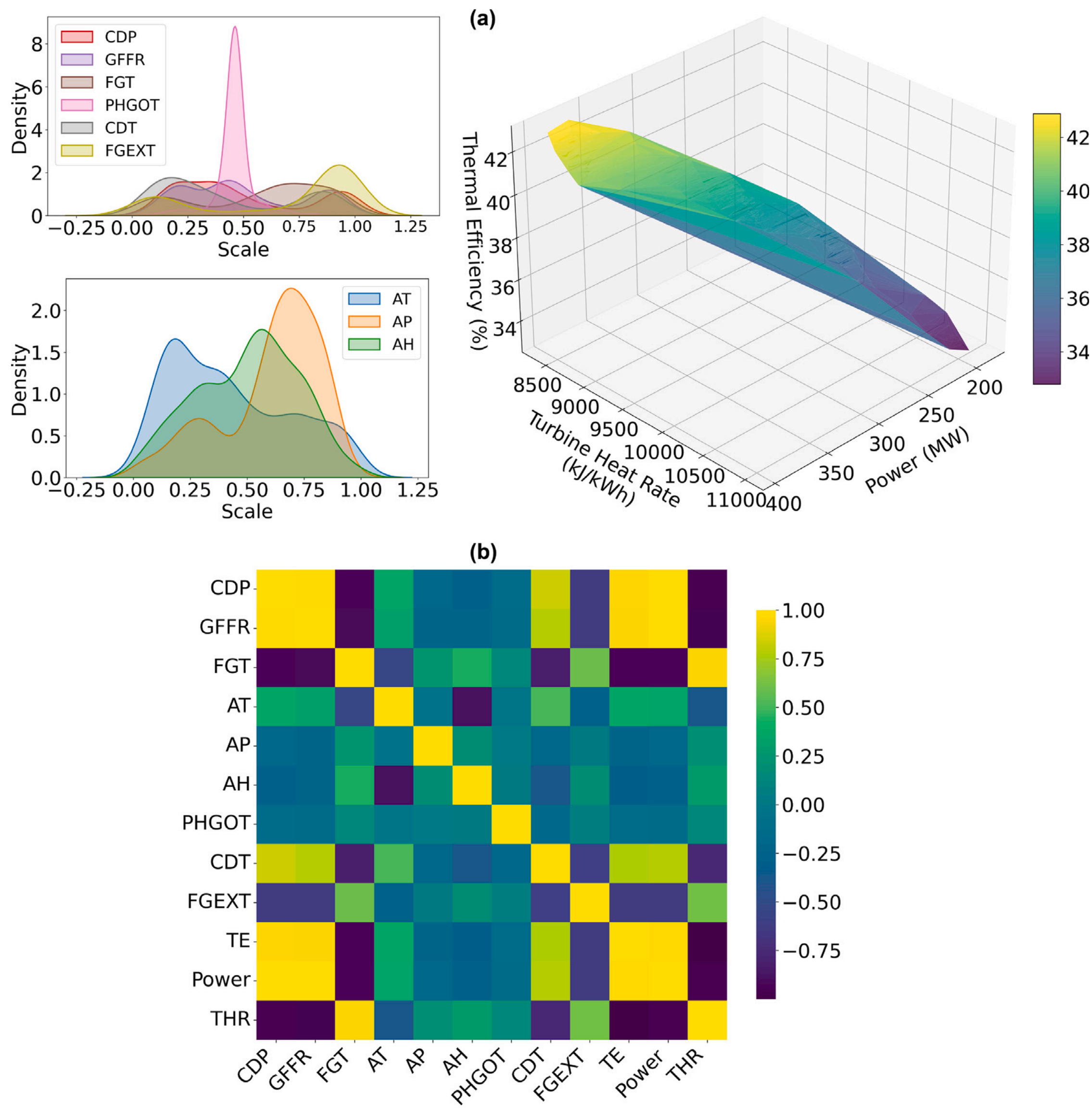

Fig. 1. Power generation from a gas turbine system. (a) Data visualization and (b) understanding the operation characteristics of system.

predicts thermal efficiency with R^2 of 0.97 and 0.96, while RMSE of 0.39% and 0.40% are obtained on the training and testing datasets, respectively. A perfect fit is observed on the training and testing data sets to predict the power (MW) on the trained ANN model (optimized hidden layer neurons are 31), measuring R^2 of 1.0, respectively.However, RMSE of 1.07 MW and 1.16 MW, respectively, are present in the predictions made by the power model in the training and testing datasets. The ANN model trained to predict the turbine heat rate has an 31 optimal number of neurons in the hidden layer, and the trained ANN model predicts the turbine heat rate with R^2 of 0.97 and RMSE of 93 kJ/kWh and 99 kJ/kWh, respectively, on training and testing data sets. The ANN models, trained to predict the three performance variables, exhibit excellent predictive performance on test datasets, which is not only comparable with those of training datasets, but is also

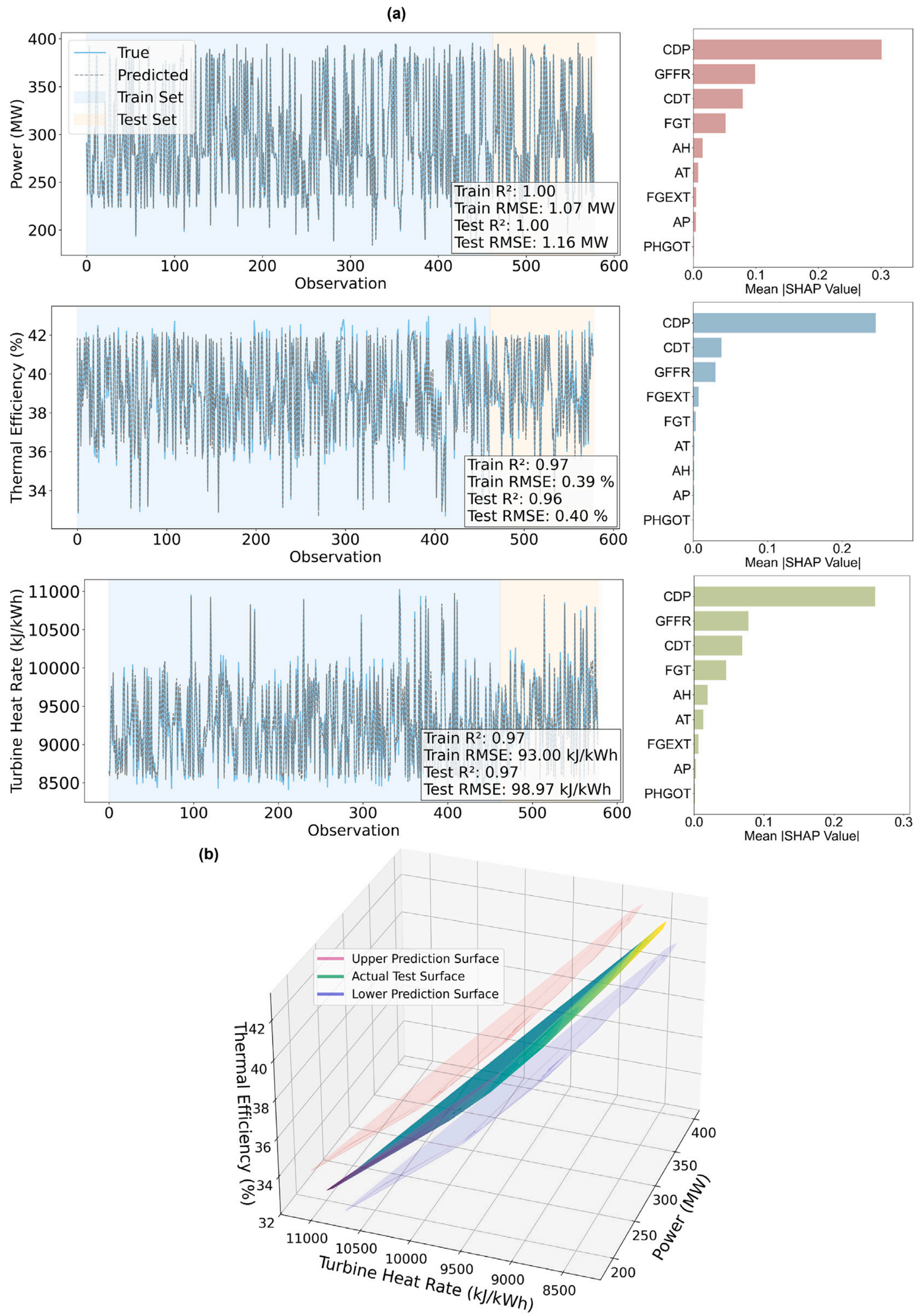

Fig. 2. Data-driven modeling of the power generation system. (a) ANN-based modeling and the associated feature importance list made by SHAP for three key performance variables (thermal efficiency, power and turbine heat rate) of the gas turbine system. (b) Mapping the test data-driven actual function space of three performance variables on estimated upper and lower prediction surfaces.

the indicator of good generalization capability induced in the trained models for the predictive tasks.

The feature importance analysis is performed by embedding the trained ANN models in the SHAP framework, and the feature importance order is established for the three performance variables. The mean SHAP values are plotted as bars corresponding to each variable and are shown on the right side of Fig. 2(a). SHAP-based analysis reveals that CDP is the most significant process variable and is followed by GFFR, which affects the thermal efficiency of a gas turbine system. However, CDP and CDT turn out to be the two significant process variables in predicting the power of the gas turbine system. Similarly, CDP and GFFR are estimated to be the two significant variables for predicting the turbine heat rate. The significance of CDP, CDT and GFFR is explainable through the operating characteristics of the gas turbine system, which are established through the power generation operation in the industrial environment. CDP and CDT are measured at the outlet of air compressors and establish the thermodynamic conditions of the airflow rate that is injected into the combustion chamber. GFFR is the amount of gas that is supplied into the combustion chamber and undergoes combustion in the presence of air. The process variables maintain and stabilize temperature of the hot flue gases, which are expanded in the gas turbine to produce power. The work potential of hot flue gases is extracted in a gas turbine, and thermal efficiency and turbine heat rate are measured to account for the energy conversion ratio and thermal energy spent to produce the power from the gas turbine system.

The prediction intervals for the predictions made by the three ANN models are computed by inductive conformal prediction technique [63]. The function space built on the observations of the test datasets of the three performance variables is constructed and is labeled as actual test surface in Fig. 2(b). The prediction intervals computed on the three performance variables are utilized to construct upper and lower prediction surfaces with a 95% confidence level. We observe that the constructed prediction surfaces enclose the actual test surface, confirming the validity of the upper and lower prediction surfaces to quantify the uncertainty associated with ANN-based predictions for the three performance variables. Moreover, the upper and lower prediction surfaces are in close proximity to the actual test surface, underscoring the excellent modeling performance of the trained ANN models to predict the performance variables of the gas turbine system. The good generalization as well as modeling performance of the trained ANN models approximate the data-driven operating characterizes of operation of the gas turbine system. Later, the trained ANN models are embedded in the optimization environment for model-based analysis as discussed in the following.

3.3. Data-centric optimization of gas turbine system

Industrial gas turbine systems are installed to supply the electrical power in the grid to meet energy demand. In the industrial environment, power supply is prioritized over thermal efficiency and turbine heat rate, since the produced power is sold to the central power purchaser. However, during power generation operations, operators also tend to maximize thermal efficiency and minimize the turbine heat rate, as these performance variables affect the cost of power generation. Therefore, we have formulated an objective function that aims to maximize thermal efficiency and minimize turbine heat rate, given that the set value of power, that is to be produced from the gas turbine system, must be satisfied. This mimics the operating scenario of the operation of the gas power plant that is ramped up or ramped down on the available capacity such that the optimal operating conditions to operate the gas turbine system are estimated on the set value of power. However, we have analyzed the formulated objective function and the constraint on power generation under two scenarios: (1) the MAD-OPT framework and (2) when we do not embed the Mahalanobis constraint into the optimization problem. Here, the purpose of analysis of these two types of optimization problem is to demonstrate how embedding and not embedding the domain-specific information into the optimization problems provide "Optimal" solutions that may or may not be implemented in the operation of the industrial systems in general and gas power plants in particular.

Fig. 3 shows the convergence of the optimization solver to the feasible optimal solution corresponding to the different initial points with respect to the set power value of 390 MW for the MAD-OPT framework (Fig. 3(a)) and when the Mahalanobis constraint is not embedded in the optimization problem (Fig. 3(b). The mapping of the optimal values of the process variables is also depicted against the contour plots which are made on the actual data of the power plant to demonstrate the domain consistency of the optimal solutions under two types of optimization problems. The empiric approach is implemented to estimate the width of the ellipse that captures the data corresponding to the pair of variables: the tighter the ellipse is, the more correlated the pair of variables are and vice versa. We have taken compressor discharge pressure and gas fuel flow rate as a correlated pair of variables to make a contour plot and to map the optimal solution in the plot. The two correlated variables are selected because they turn out to be the significant variables affecting the power generation from the gas turbine system. Similarly, a weakly correlated pair of variables, compressor discharge temperature & performance heater gas outlet temperature, is selected to visualize how optimal solutions would be mapped against the contour plot made in the actual data of the gas power plant.

It is important to mention earlier that we have set the tighter bounds on variables related to ambient conditions near the mean values estimated from the actual data of the power plant. This allows to incorporate real-time ambient conditions corresponding to the set value of power of 390 MW in the optimization problems in order to determine the optimal values of process variables. The tighter bounds on the ambient conditions allow simulating an industrial operating scenario corresponding to nearly fixed ambient conditions when capacity discharge of the gas turbine system is going to be changed at a particular instant of time. The tolerance on the Mahalanobis distance is set to 0.9, which serves as a feasible region for the optimization solver to estimate the solution.

Fig. 3(a) displays the optimal values of gas fuel flow rate (47.4 lb/s), turbine heat rate (8447 kJ/kWh), and thermal efficiency (43.02%) corresponding to a set power value of 390 MW, which are estimated by the MAD-OPT framework. The optimal values of the turbine heat rate and thermal efficiency are estimated to be within their operating limits, which were established corresponding to plant's operation. It is also apparent that the estimated optimal solutions for the process variables are mapped within the ellipses, confirming the efficacy of the solutions in terms of their implementation in the operation of the gas turbine system.

Referring to Fig. 3(b), although the optimization solver achieves a feasible solution on the set power of 390 MW; the optimal values of turbine heat rate (6793 kJ/kWh) and thermal efficiency (47.80%) are significantly beyond the operating limits of these two performance variables, as mentioned in Table 1. The solver estimates these optimal values corresponding to the gas fuel flow rate of 28.56 lb/s which is its minimum operating value during the plant's operation. The anomalous optimization results obtained without the Mahalanobis constraint can be identified by visualizing the mappings of optimal solutions related to process conditions in the contour plots made in Fig. 3(b). The obtained optimal solutions lie outside the operating envelopes which indicate the unsafe aspect of optimal solutions, violating the dependencies among the process variables and may potentially jeopardize the process safety. Although trained ANN models demonstrated good predictive performance on the test datasets; the integration of parametric ANN models with a "goal-oriented" and "greedy" optimization solver may result in the estimation of a "feasible" optimal solution which may not satisfy the variable correlation structures that may have been mapped during the training of the ANN models. This potential caveat in deploying the AI models for estimating the optimal solutions can be a barrier in the AI-adoption in industrial setting which can be overcome through embedding Mahalanobis distance-based constraint in the optimization problem.

3.3.1. Stress test—Ramping up the power generation from gas turbine system

We also estimate the optimal process conditions when power generation from a gas turbine system is increased from 185 to 395 MW with a

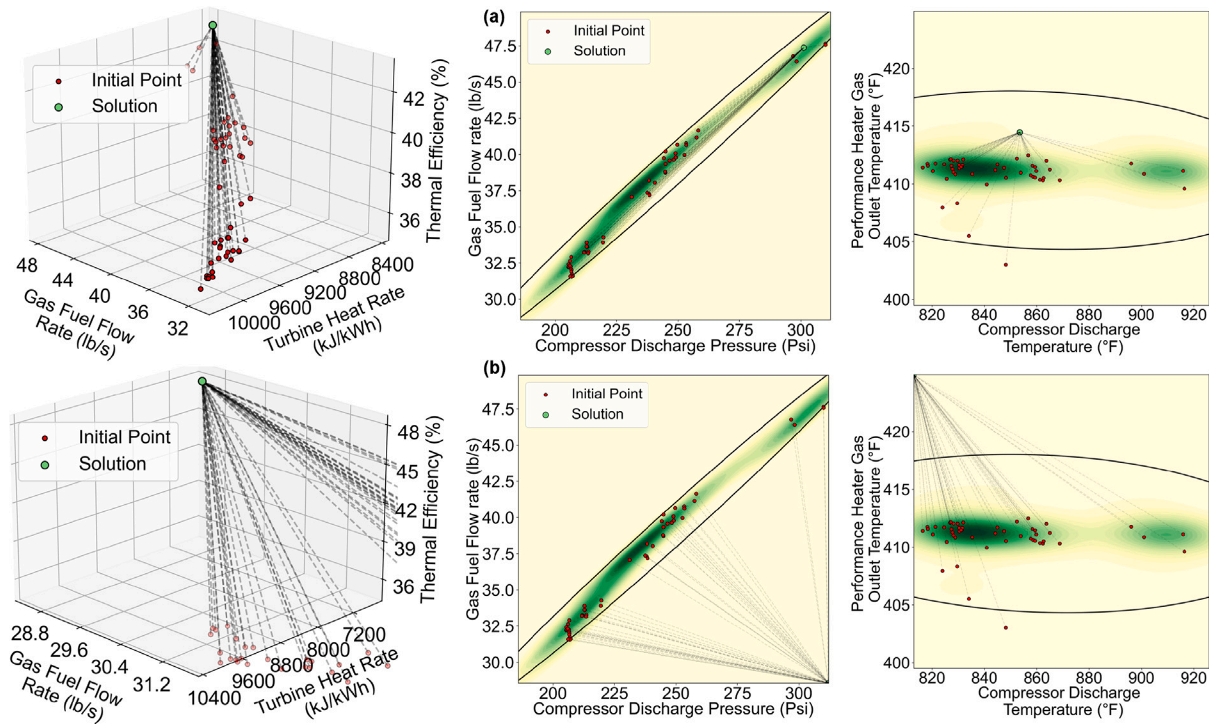

Fig. 3. Solving an optimization problem and mapping the optimal solutions for a power set point of 390 MW by (a) the MAD-OPT framework and (b) when the Mahanalobis constraints are not embedded in the optimization problem. The yellow-region depicts the operating bounds of the process variables.

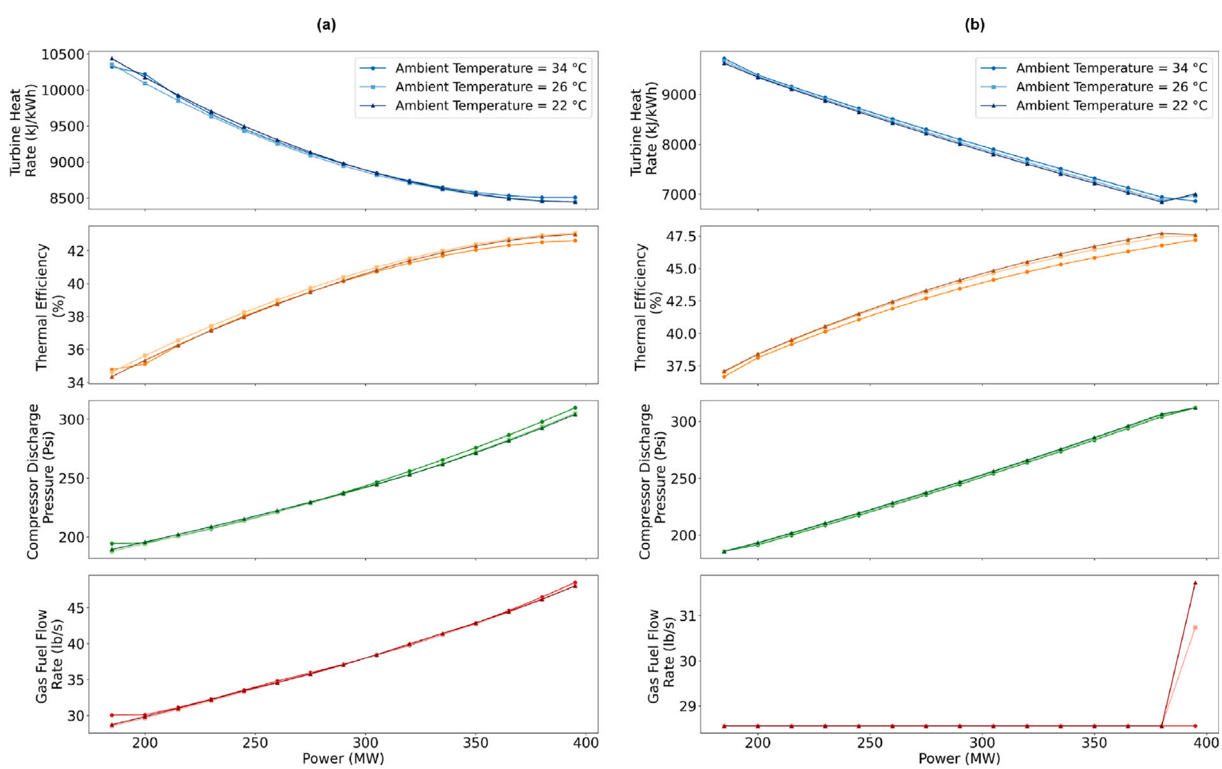

Fig. 4. Performance curves obtained on solving the optimization problem for power ramp-up operation of the gas turbine system by (a) the MAD-OPT framework and (b) when the Mahalanobis constraints are not embedded.

step size of 15 MW. The ramping-up operation is simulated in three sets of ambient conditions, with ambient temperatures of 22 °C (minimum), 26 °C (average) and 34 °C (maximum) taken from the actual data of the gas power plant operation. We also analyze how the integration of the Mahalanobis constraint affects the efficacy of optimal solutions in terms of their domain consistency. Fig. 4 compares the solutions profiles estimated during the operation of the increase in power under three different ambient conditions corresponding to (a) the MAD-OPT framework and (b) no integration of the Mahalanobis constraint in the optimization problems.

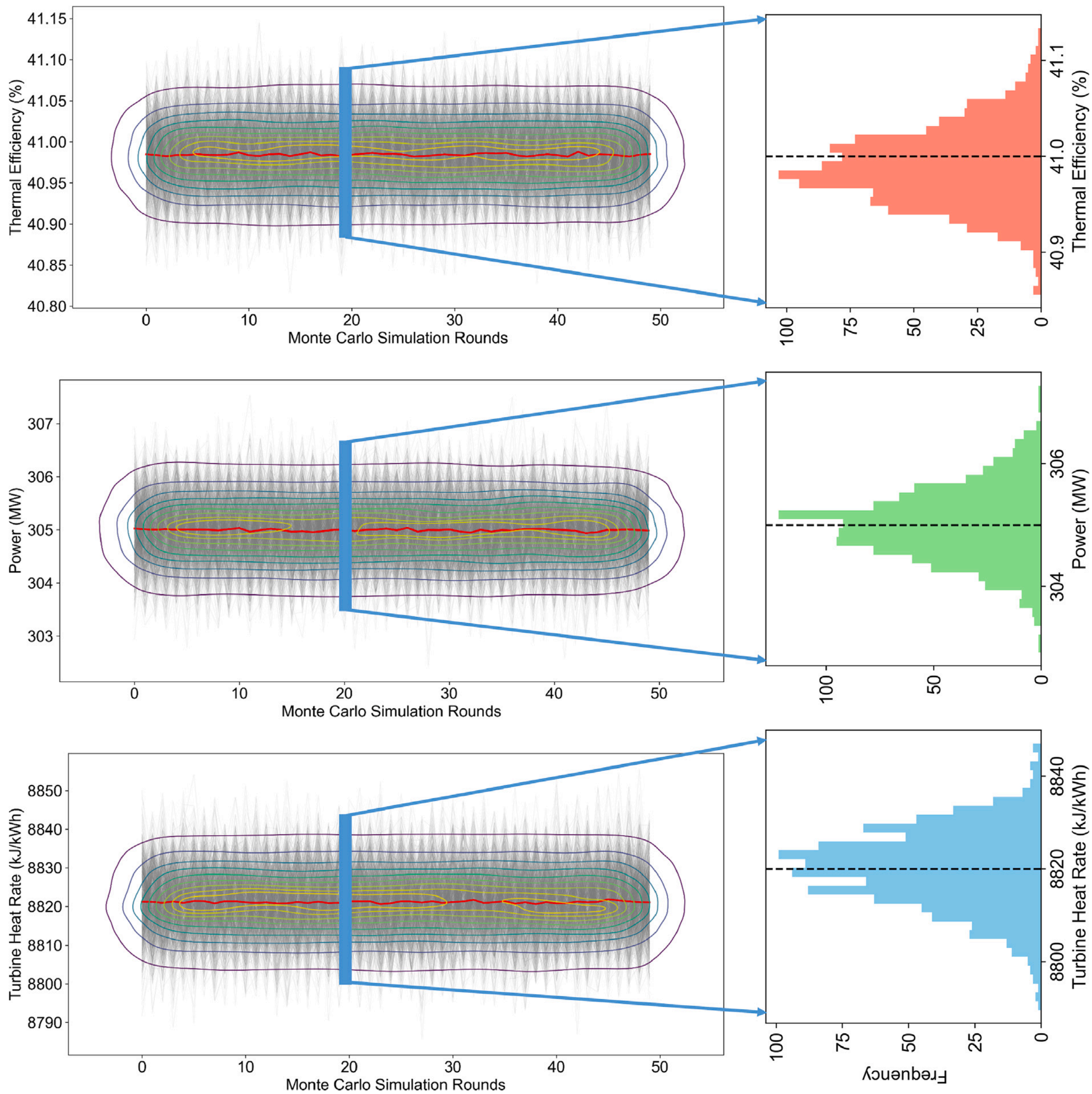

Fig. 5. Evaluating the robustness of the optimal solutions obtained through ANN models.

Referring to Fig. 4(a), we notice a smooth and increasing trend in compressor discharge pressure and thermal efficiency, whereas a decreasing trend in turbine heat rate when the power set point increases from 185 MW to 395 MW. Thermal efficiency of the gas turbine system is increased from 34.35% to 42.99% and 34.77% to 42.60% corresponding to the ambient temperatures of 22 °C and 34 °C respectively on ramping up the power. It is important to note here that, overall, thermal efficiency of the gas turbine system is decreased by 0.1% when operated at 34 °C in comparison to the full power ramp-up turbine's operation at 22 °C. Similarly, gas fuel flow rate is found to be decreased by 0.18 lb/s on operating the gas turbine system at 22 °C as compared to its operation at 34 °C during the power ramp-up.

Although we notice smooth and increasing trends for compressor discharge pressure and thermal efficiency, with a decreasing trend for turbine heat rate when power ramp-up operation is optimized without embedding the Mahalanobis constraint into the optimization problem as shown in Fig. 4(b). The optimization solver consistently estimates 28.56 lb/s as an optimized value of the gas fuel flow rate for almost all set points of power under three ambient conditions. This anomalous value of gas fuel flow rate clearly indicates the domain-inconsistent performance of parametric ANN models when embedded in the optimization problems which lack in the integration of domain knowledge. These results reinforce the need to embed domain-informed data-driven constraints into the optimization problems that guide the solver during the solution-search phase for estimating a truly "feasible" and "domain-informed" solution for the optimization problem. Thus, merely relying on the input–output mappings within the ANN model is not sufficient to estimate effective optimal solutions for the optimization problems. The quantification of data patterns and their introduction as constraints in the optimization problem synergizes with the capabilities of ANN models to accelerate the estimation of domain-informed optimal solutions that may enhance the operational excellence of industrial systems.

3.3.2. Robustness evaluation of the optimal solutions

Fig. 5 shows the variation in the optimal values of thermal efficiency and turbine heat rate corresponding to the set value of power. A mean response is calculated in each simulation round and plotted to visualize its variation across the simulation rounds. A contour plot

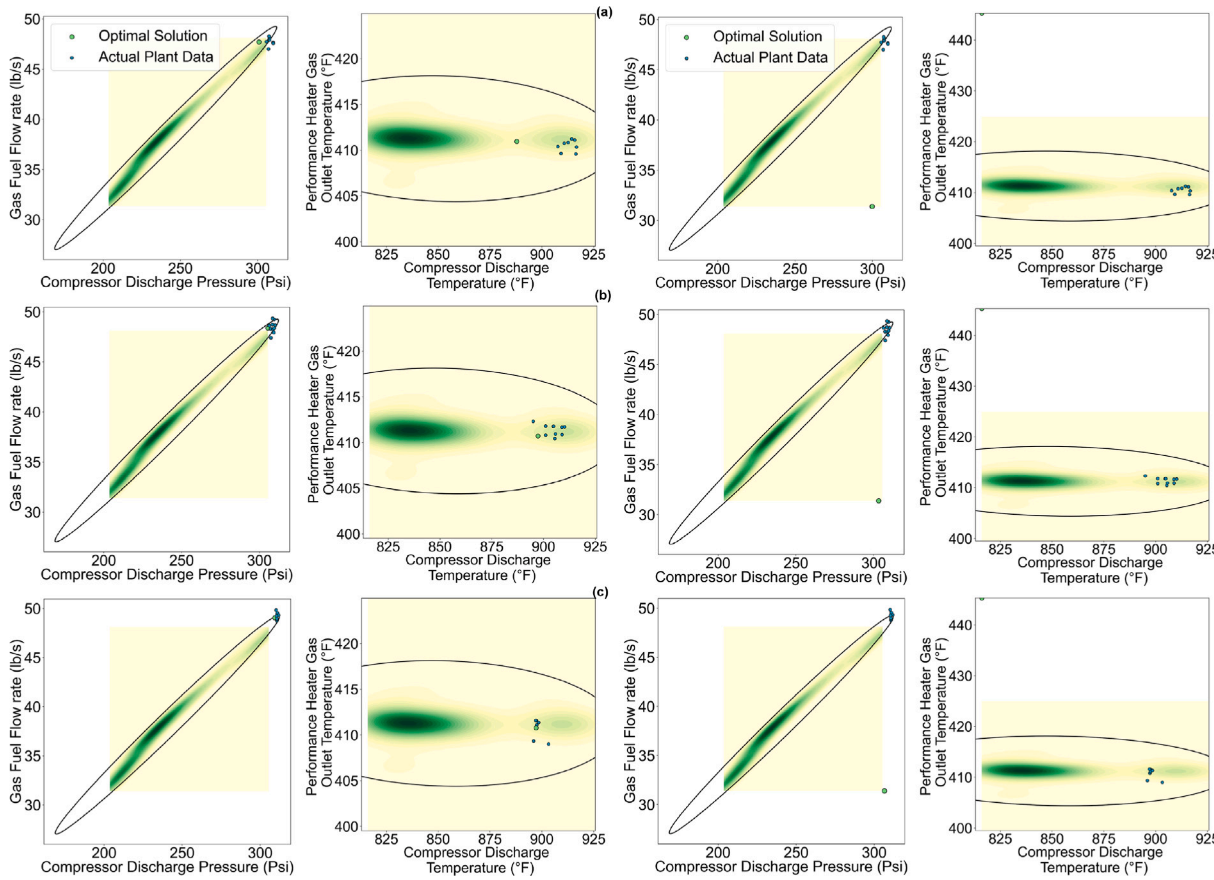

Fig. 6. Extrapolating ANN models for producing power beyond the design limit of gas turbine system. The optimization problem is solved with and without the Mahalanobis constraint, and the solutions are mapped for the set values of power of (a) 385 MW, (b) 390 MW, and (c) 395 MW. The pair of plots on the left side corresponds to the extrapolation results obtained by the MAD-OPT framework. The yellow-shaded rectangles depict the operating bounds of the process variables.

is also made to visualize the data distribution density for the rounds of simulations. We observe a fairly flat mean response for three performance variables that is quite close to the deterministic solutions, i.e., thermal efficiency = 40.98%, power = 305 MW and turbine heat rate = 8820 kJ/kWh. The mean response and confidence interval in the highlighted round of Monte simulations are calculated as: thermal efficiency = 40.99 ± 0.16%, power = 304.98 ± 2.20 MW, turbine heat rate = 8820 ± 32.81 kJ/kWh. The confidence intervals computed on the perturbed inputs for the three performance variables appear to be tight, demonstrating that the estimated solution is fairly robust to the perturbation in the process input variables.

3.4. Operating beyond the designed capacity

The ANN models are trained on a subspace of actual data and predict power, thermal efficiency, and turbine heat rate on the test dataset using the following performance metrics: $(R^2 = 1.0, \text{RMSE} = 1.50\ \text{MW})_{\text{Power}}$, $(R^2 = 0.95, \text{RMSE} = 0.46\%)_{\text{Thermal Efficiency}}$ and $(R^2 = 0.96\ \text{MW}, \text{RMSE} = 103\ \text{kJ/kWh})_{\text{Turbine Heat Rate}}$. We observe comparable modeling performance of the trained ANN models on the subspace of actual data as compared to full-space's modeling results reported in the previous section.

We use the same optimization problem formulation as utilized previously and set the power values of 385 MW, 390 MW, and 395 MW separately for two types of optimization problems: (a) when the Mahalanobis constraint is embedded (MAD-OPT framework) and (b) when the Mahalanobis constraint is not embedded in the optimization problem for extrapolating ANN models. During extrapolation, our objective is to maximize thermal efficiency and minimize turbine heat rate while estimating the optimal process conditions which satisfy the constraint of a set value of power. We set the upper bounds of the process variables to 1.8 (on a scaled basis) since producing power beyond the design limits may require higher values of the process variables. Moreover, we use the mean values of ambient conditions and slightly perturb them, since these conditions remain nearly constant when power is ramped up or ramped down at the particular instant of time.

Fig. 6(a–c) compares the optimization-based extrapolation performance evaluation of the trained ANN models corresponding to the set values of power of 385 MW, 390 MW, and 395 MW, respectively. The optimization problem is solved using the MAD-OPT framework, and the optimal solution mappings are shown on the left side of Fig. 6. We tune the tolerance parameter related to the Mahalanobis constraint during the extrapolation analysis since it controls the feasible space that the solver can explore during the estimation of solutions. Setting a high tolerance value in combination with large limits on process variables may result in out-of-ellipse mappings of optimal solutions, which will be impractical to implement in the gas turbine system. We fixed the upper bounds of the process variables and tried different values of the tolerance parameter linked to the Mahalanobis constraint such that the set value of the power constraint is satisfied and the optimal solution is mapped within the ellipses of the pair of variables, as shown on the left side of Fig. 6(a–c). The optimal value of the tolerance parameter is estimated to be 0.4, 0.45 and 0.6, corresponding to set values of power of 385 MW, 390 MW and 395 MW, respectively. These values are estimated based on the in-ellipse mappings of optimal solutions, as well as satisfaction of the set-power constraint that reflects confidence

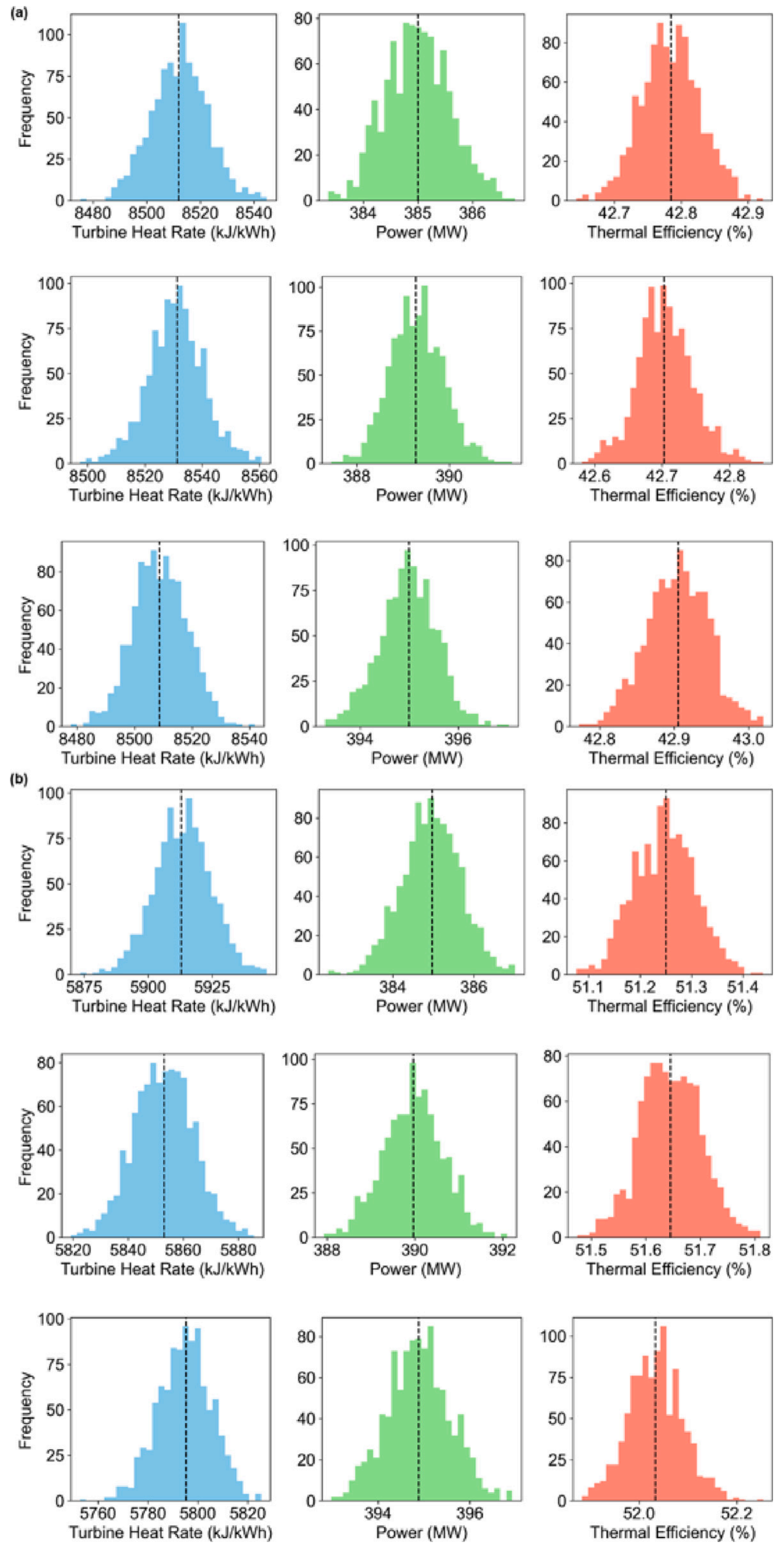

Fig. 7. Quantifying the robustness of extrapolated solutions corresponding to set values of power of 385 MW, 390 MW and 395 MW by (a) the MAD-OPT framework and (b) when the Mahalanobis constraint is not embedded in an optimization problem.

in extrapolating the neural network with the domain information and variable dependencies captured through the Mahalanobis constraint.

We also compare the optimal values of the process conditions with the corresponding actual values of process conditions that we had already separated during sub-space sampling from the actual data of the gas turbine system. The comparison reveals that compressor discharge pressure and gas fuel flow rate need to be set at higher values while producing power above the design limit (380 MW). The yellow-shaded rectangle is the subspace of the two process conditions on which ANN models have been trained. The optimal solutions corresponding to the set power values of 385 MW, 390 MW, and 395 MW lie not only outside the subspace, but also close to the actual data of the gas turbine system, which serve as ground truth to verify the accuracy of the extrapolation analysis. However, the optimal solutions estimated for compressor discharge temperature and performance heater gas outlet temperature remain in-ellipse under three set values of power and are not extrapolated beyond the subspace. This can be attributed to the low significance of these process variables in ANN-based predictions and the weak correlation between them, which makes them set at operating levels such that their correlation structure is satisfied.

We also estimate the optimal process conditions for extrapolating the power generation from the gas turbine system such that the Mahalanobis constraint is not embedded in the optimization framework. Under such conditions, the mappings of the optimal solutions are made and are shown on the right side of Fig. 6(a–c) corresponding to the set values of power of 385 MW, 390 MW and 395 MW, respectively. The optimal solutions for correlated pairs of variables are mapped outside the ellipse, and interestingly, the solver does not enable the ANN to extrapolate well even though the upper bounds on the process variables were set to 1.8, the same as the Mahalanobis constraint-based extrapolation analysis. Similarly, the optimal values of the weakly correlated pair of process variables are mapped significantly outside their subspace region and seem not to follow the structure of the variable dependencies. These results indicate that the MAD-OPT framework can enable the ANN models to extrapolate, meaning gas turbine systems can be operated slightly outside the design space. These findings demonstrate the ability of the MAD-OPT framework to adapt with the operating scenarios of industrial operations of gas turbine system and can accelerate the AI-adoption rate in safety-critical industrial systems.

3.4.1. Robustness evaluation of ANN-based extrapolated solutions

We apply the same methodology for the robustness evaluation of optimal solutions using Monte Carlo simulations. The only difference is the noise level, which is taken as 1.2% of the standard deviation of the actual data associated with the process variables of the gas turbine system. A relatively larger noise level can cover a wide space around the optimal solution and evaluate the sensitivity of the optimal solutions to the perturbations in the process conditions. The confidence intervals are calculated for the robustness evaluation of extrapolated solutions.

Fig. 7 compares the Monte Carlo simulations-based distributions of responses around the deterministic solution estimated by (a) the MAD-OPT framework and (b) the Mahalanobis constraint is not embedded in the optimization problem. The confidence intervals are also calculated for the extrapolated set values of power of 385 MW, 390 MW, and 395 MW. Referring to Fig. 7(a), mean turbine heat rate is changed from 8512 ± 40 kJ/kWh to 8508 ± 36 kJ/kWh, power is varied from 385 ± 2.2 MW to 395 ± 2.2 MW and the thermal efficiency is increased from 42.78 ± 0.17% to 42.90 ± 0.16%. The confidence intervals are fairly tight, and the estimates are based on the perturbed process variables. We also compute the confidence intervals on the optimal solutions when estimated without the Mahalanobis constraint. Although the optimal values of thermal efficiency and turbine heat rate are significantly away from their operating ranges, we observe relatively higher confidence intervals on their estimates. We computed the confidence interval of 42 kJ/kWh, 42 kJ/kWh and 41 kJ/kWh for the turbine heat rate, 2.8 MW, 2.6 MW and 2.7 MW for power, and 0.22%, 0.22% and 0.23% for thermal efficiency, corresponding to set power values of 385 MW, 390 MW and 395 MW, respectively. The relatively higher confidence intervals computed for extrapolated solutions without the Mahalanobis constraint may be attributed to solutions convergence significantly away from the trained space of ANN models, and models may exhibit higher sensitive responses, leading to relatively larger confidence intervals than those of solutions estimated closer to the trained space of ANN models.

The systematic comparison of optimization-based extrapolation analysis carried out with and without the integration of domain-specific information reveals that ANN models can be made to extrapolate with reasonable accuracy and exhibit lower predictive uncertainty, which stems from following the variable dependencies that exist in the data. The challenge remains to identify data-driven constraints that effectively capture domain knowledge. However, domain-knowledge constrained optimization problems can be a way forward towards AI adoption for the operation excellence of the gas turbine system. This research supports operation excellence and sustainability principles by enhancing thermal power plant efficiency and reducing turbine heat rate through domain-informed AI optimization, enabling safer, more reliable, and energy-efficient operations that remain robust under varying conditions and adaptable beyond design limits [64]. Moreover, this research also contributes to the United Nations Sustainable Development Goals of Industry, Innovation and Infrastructure (goal # 9) and compliments Affordable and Clean Energy (goal # 7).

4. Conclusion

This study demonstrates the successful development and implementation of the MAD-OPT framework for optimizing gas turbine operations, addressing the critical challenge of the adoption of AI in safety-critical industrial systems. The effectiveness of the MAD-OPT framework is evidenced by the ANN models that achieve a prediction accuracy of more than 95% for power, thermal efficiency and turbine heat rate, with reliability confirmed by uncertainty analysis based on inductive conformal prediction. SHAP analysis identified compressor discharge pressure, compressor discharge temperature, and gas fuel flow rate as significant operational determinants. Under varying ambient conditions, the framework revealed that the increase in power from 185 MW to 395 MW yielded a 0.1 percentage point increase in thermal efficiency at 22 °C compared to 34 °C. Moreover, robust optimal values of 40.99 ± 0.16% for thermal efficiency and 8820 ± 32.81 kJ/kWh for turbine heat rate at 305 MW are estimated at ambient temperature of 26 °C. The MAD-OPT framework also successfully extrapolated beyond the 380 MW limit of the training data to estimate process conditions at 385–395 MW, while maintaining domain consistency through the Mahalanobis constraint, a feature absent from conventional optimization approaches. The domain-compliance of the AI-driven optimal solutions as well as successful extrapolation of AI models beyond the design limit of gas turbine system are the key strengths of the MAD-OPT framework, which has demonstrated its adaptability with the operating constraints of industrial operations. Moreover, the results establish MAD-OPT as a promising framework to accelerate the safe adoption rate of AI in safety-critical industrial applications, promote energy-efficient power generation, and contribute to sustainable development goals.

Limitations and future work

The MAD-OPT framework is built on the Mahalanobis distance-based constraint and the ANN models, which is the main limitation of this research. In the future, innovative and purely data-driven constraints can be developed that quantify the nonlinear dynamics of the system from the data and are embedded in optimization problem. Moreover, the effect of different AI models on the quality of solutions under the same constraints can also be investigated.

CRediT authorship contribution statement

Waqar Muhammad Ashraf: Writing – original draft, Validation, Software, Methodology, Formal analysis, Data curation, Conceptualization. **Amir H. Keshavarzzadeh:** Writing – original draft, Validation. **Abdulelah S. Alshehri:** Writing – review & editing, Methodology, Funding acquisition, Conceptualization. **Abdulrahman bin Jumah:** Writing – review & editing, Methodology, Funding acquisition, Conceptualization. **Ramit Debnath:** Writing – review & editing, Validation. **Vivek Dua:** Writing – review & editing, Project administration, Conceptualization.

Declaration of competing interest

The authors declare no competing financial benefits and personal relationships have influenced the findings of the paper.

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Data availability

Data will be made available on request.

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