

Accelerating domain-compliant AI adoption in industrial operations: A case of combined cycle gas power plant

Waqar Muhammad Ashraf^{1,2}, Talha Ansar³, Abdulah S. Alshehri⁴, Muhammad Akhtar³, Ghulam Moeen Uddin³, Ramit Debnath², Vivek Dua¹

¹ Department of Chemical Engineering, University College London, London, UK

² Collective Intelligence & Design Group, University of Cambridge, Cambridge CB2 1PX, UK

³ Department of Mechanical Engineering, University of Engineering and Technology, Lahore 54000, Pakistan

⁴ Chemical Engineering Department, College of Engineering, King Saud University, P.O. Box 800, Riyadh 11421, Saudi Arabia

Problem Statement

- Neural networks are universal function approximators but black-box [1]
- Embedding AI models into standard optimisation framework provides domain-inconsistent solutions, not implementable in industry [2]
- Extrapolation beyond design conditions yields uncertain predictions, rendering models unfit for scaling performance [3]

Objectives

- Develop domain-constrained and data-driven robust optimisation framework with Mahalanobis trust regions
- Verify the optimal solutions against the power plant data [4]
- Domain-guided extrapolation of ANN beyond design conditions
- Development of open-source neural simulation platform

Method

Domain-consistent optimisation framework [5]:

- Domain-constrained robust optimisation problem is defined for multi-level operation of combined cycle gas power plant:

$$\begin{aligned} \min_x f(x) &= -f_{TE}(x) + f_{THR}(x) \\ h(x) &= 0 \\ (f_{Power}(x) - Power_{SetPoint})^2 &< \epsilon \\ (x - \mu)^T \Sigma^{-1} (x - \mu) &< \tau^2 \\ f_{Power}(x) - \sum_{i=1}^3 x_i &< \Delta \\ x^L &\leq x \leq x^U \end{aligned} \quad (1)$$

Here, thermal efficiency (TE) and turbine heat rate (THR) are the plant-level performance metrics which are optimised against $Power_{SetPoint}$

- The robustness of the optimal solution (x^*) is evaluated by variance ($V(x^*)$) produced in multi-objective function due to input perturbation (δ_k):

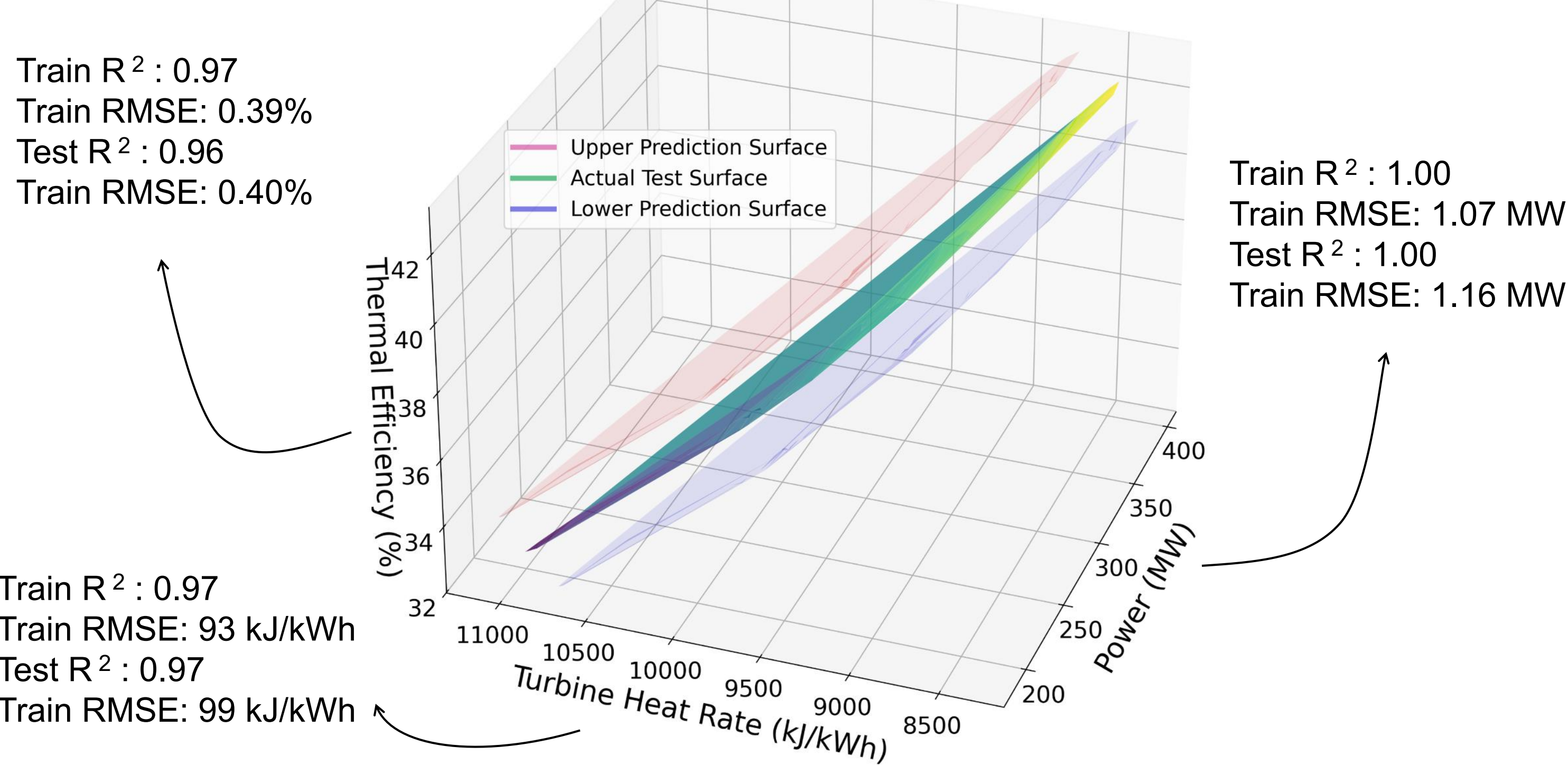
$$\begin{aligned} F(x^*) &= \frac{\sum_{k=1}^H f(x^* + \delta_k)}{H} \\ V(x^*) &= \frac{\|F(x^*) - f(x^*)\|}{\|f(x^*)\|} < \epsilon \end{aligned} \quad (2)$$

Extrapolation of ANN model

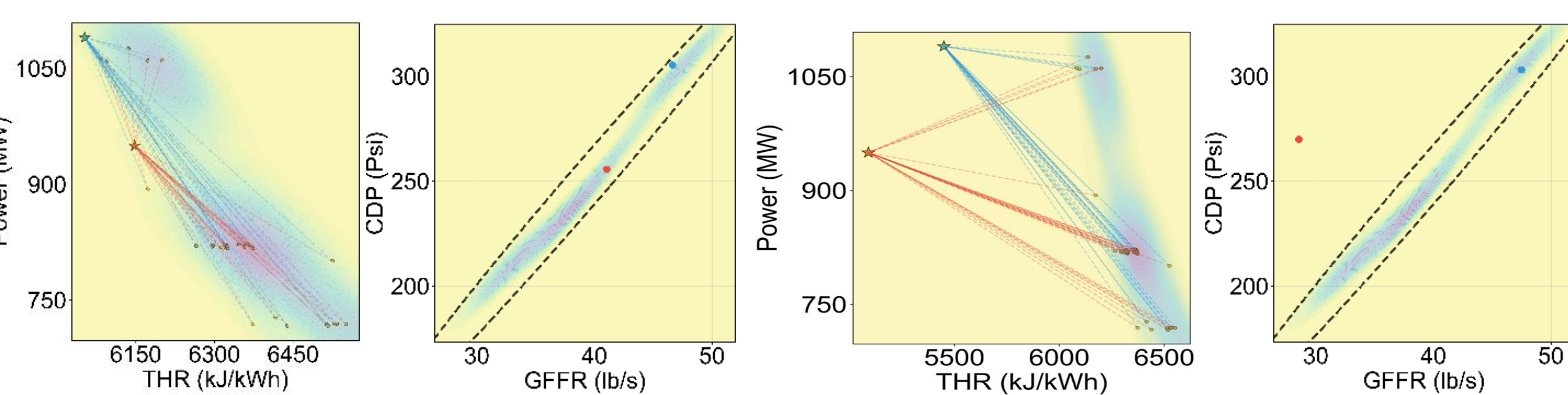
- ANN models are trained on **subsample** of dataset
- Extrapolation is carried out with optimisation problem (1)

Open-Source Neural Simulation Platform: A case of combined cycle gas power plant

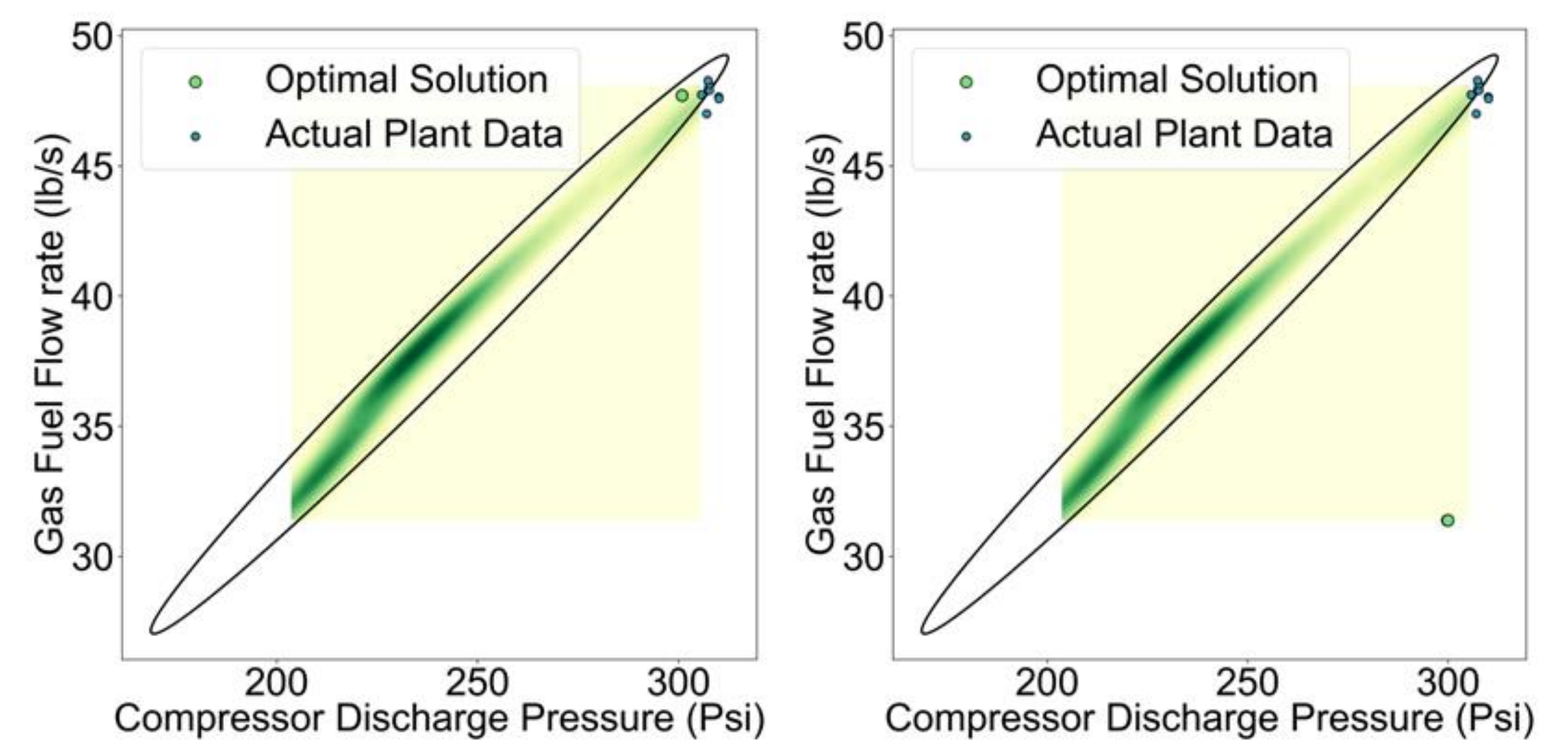
- Three-layer ANN models are trained for performance variables, Power (MW), TE, THR of 395 MW capacity gas turbine



- The optimal solutions are compared, estimated **with** and **without** Mahalanobis constraint for 1180 MW capacity gas power plant



- ANN is trained on data ≤ 380 MW, with 381–395 MW retained as **ground truth** for extrapolated results



- An open-source **explainable and uncertainty-aware simulation platform** for **real-time process optimisation** is developed

Neural Simulation Platform

$Power_{SetPoint}$ 350
Tolerance 80 } Input

Power: 350 ± 2 MW
Thermal Efficiency: 42.10 ± 0.08 %
Heat Rate: 8465 ± 38 kJ/kWh } Output



Conclusions & Future Work

- Data-driven industrial domain knowledge** is quantified by Mahalanobis distance
- Solving the domain-constrained optimisation problems provides implementable solutions for **existing control layer** of industrial systems
- Domain-knowledge can help **safely extrapolate** ANN models for industrial applications
- Neural simulation platform adapts with **industrial constraints** and carries **real-time process optimisation**
- Future work on generalised framework on **model adaptation** with data drift and evolving process conditions

References

- M. Rätz, P. Henkel, P. Stoffel, R. Streblow, and D. Müller, "Identifying the validity domain of machine learning models in building energy systems," *Energy and AI*, vol. 15, p. 100324, 2024.
- Benítez, José Manuel, Juan Luis Castro, and Ignacio Requena. "Are artificial neural networks black boxes?." *IEEE Transactions on neural networks* 8, no. 5 (1997): 1156-1164
- Brynjolfsson, Erik, and A. N. D. R. E. W. McAfee. "Artificial intelligence, for real." *Harvard business review* 1 (2017): 1-31.
- IEA (2025), Energy and AI, IEA, Paris <https://www.iea.org/reports/energy-and-ai>, Licence: CC BY 4.0
- Ashraf, Waqar Muhammad, Amir H. Keshavarzzadeh, Abdulelah S. Alshehri, Abdulrahman bin Jumah, Ramit Debnath, and Vivek Dua. "Domain-Informed Operation Excellence of Gas Turbine System with Machine Learning." *arXiv preprint arXiv:2507.08697* (2025).

