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Machine Learning–Based Surrogate Modeling for Performance Evaluation in Energy-Aware Reconfigurable Manufacturing Systems

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Abstract: In the context of Industry 4.0, manufacturers must adapt rapidly to fluctuating demand while minimizing energy consumption. Although Reconfigurable Manufacturing Systems (RMS) provide flexibility, performance evaluation still relies on computationally intensive simulation, limiting fast reconfiguration decisions. This study proposes a machine learning surrogate modeling framework to provide fast and accurate performance estimates for a set of RMS configurations. A dataset of 372 demand-driven scenarios across three configurations was generated using a forecast-driven reconfigurable cyber-physical production system. Near-optimal schedules were obtained via a genetic algorithm integrated with discrete-event simulation. Twelve machine learning models were evaluated to predict three targets: Mean Flow Time, Total Energy Consumption, and a normalized multi-objective fitness score. The optimal models achieved near-perfect estimation capabilities, characterized by a mean absolute percentage error of approximately 0.20% for Mean Flow Time, 0.02% for Total Energy, and 12% for the fitness score, while maintaining inference times under 4 ms per scenario. These results demonstrate that machine learning can effectively construct surrogate models for predicting system performance, enabling real-time and energy-aware evaluation to support adaptive RMS reconfiguration, accelerating the process by 10^5 compared to exhaustive simulation-based search.

Keywords: Reconfigurable Manufacturing Systems, Surrogate Modeling, Machine Learning, Simulation-Based Optimization, Energy Efficiency, R-CPPS.

1. INTRODUCTION

Originating as a response to globalization, Reconfigurable Manufacturing Systems (RMS) combine the advantages of dedicated serial lines and flexible manufacturing systems to maximize responsiveness to fluctuating demand. By design, RMS aims to be cost-effective: it boosts productivity and prolongs the manufacturing system's lifetime by allowing continuous adaptation to unforeseen market changes (Koren et al., 2018). Unlike Dedicated Manufacturing Lines, RMS allows for the rapid addition, removal, or rearrangement of machine modules to adjust capacity and functionality. Crucially, this adaptability also serves the growing imperative for sustainable manufacturing. By aligning production resources precisely with demand, RMS can potentially minimize idle times and optimize energy consumption, addressing the dual challenge of productivity and environmental footprint.

In this context, production scheduling and workforce planning constitute two essential operational challenges in an RMS, both aiming to optimize the allocation of manufacturing resources over a defined planning horizon. Given a predefined set of system configurations, scheduling within an RMS requires determining the sequence in which configurations are "activated" as well as assigning operations to their corresponding processing intervals. Operation processing times are expected to vary depending on the chosen configurations (Ostovari et al., 2024). However, realizing this potential introduces significant complexity in process planning. Determining the optimal system setup is not merely a matter of hardware selection; it requires solving two interdependent problems simultaneously: defining the physical system configuration and optimizing the logical production schedule. Thus, evaluating the performance of a specific RMS configuration therefore typically requires Simulation-Based Optimization (SBO), where a metaheuristic generates candidate solutions that are evaluated by a Discrete Event Simulator (DES). While SBO provides accurate performance estimation and systematically searches for optimal configurations through repeated simulation runs, it suffers from a critical limitation in its high computational cost. Running detailed simulation-based optimization for all potential configuration scenarios, especially under uncertain demand patterns, is time-prohibitive. This computational overhead makes exhaustive evaluation impractical, limiting the applicability of conventional SBO approaches. Furthermore, operational

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environments often require rapid responsiveness while also demanding in-depth scenario exploration in order to effectively handle variations.

To address this issue, this paper proposes a Machine Learning (ML)–based approach grounded in surrogate modeling. Instead of executing costly simulations for every new decision, the simulator is replaced with a data-driven approximation model. We leverage system architecture and forecasting data from recent work on sustainable R-CPPS (Bouazza and Kantasa-Ard, 2025) to train ML models for predicting key performance indicators, specifically *Mean Flow Time* and *Total Energy Consumption*, as well as a *normalized weighted fitness score* aggregating multiple objectives. This approach bridges the gap between accurate but slow offline simulation and the need for fast, energy-aware configuration assessment, enabling near real-time performance estimation. This work introduces a unified ML framework for building surrogate models to rapidly evaluate RMS performance under uncertainty and multiple system configurations.

The paper is organized as follows. Section 2 reviews the state of the art, while Section 3 formalizes the problem and reference architecture. Section 4 details the proposed framework, covering data generation and model training. Experimental results are analyzed in Section 5. Finally, Section 6 concludes the paper and highlights directions for future research.

2. STATE OF THE ART

2.1 Simulation-Based Optimization in RMS

Simulation-Based Optimization (SBO) has become a common methodology for RMS performance evaluation and configuration selection, particularly because layout, assignment, and scheduling decisions are often NP-hard. Most studies therefore combine metaheuristics with Discrete Event Simulation to capture stochastic behavior and evaluate dynamic KPIs such as flowtime and throughput. However, RMS flexibility increases optimization complexity, often requiring thousands of simulation runs. For example, Renna (2024) used simulation to evaluate reconfiguration policies for integrating multi-spindle reconfigurable machines, showing that balanced machine distribution improves system performance. Similarly, Diaz et al. (2021) addressed the scaling of multi-part flow lines under uncertainty using NSGA-II-based simulation optimization, jointly maximizing throughput and minimizing buffer capacity to support efficient production ramp-up.

Other studies focus specifically on layout optimization. For example, Wang et al. (2024) introduce a dynamic layout optimization framework driven by a high-fidelity 3D simulation environment. By constructing a digital twin within visual components controlled, the authors replace traditional 2D approximations with realistic 3D facility models. This simulation serves as a training ground for a decentralized multi-agent cooperative swarm learning algorithm, enabling the system to optimize layouts while accurately accounting for physical constraints such as robot reachability and collisions. Kazemisaboor et al. (2021) propose a two-step framework for process plan generation in RMS to ensure adaptability to unpredictable market changes. The first step addresses single-unit process plan generation by comparing three metaheuristics with simulation-based optimization. The second step focuses on multi-unit process plan generation for varying demand periods, introducing a novel heuristic named the designed periods algorithm alongside NSGA-II for unit optimization.

Recent work extends these approaches by introducing sustainability objectives, such as energy consumption and emissions. For example, Khettabi et al. (2021) address the challenge of designing sustainable RMS that balance cost-effectiveness with environmental constraints. To solve the multi-objective problem of selecting sustainable machines and tools, the authors formulate a non-linear multi-objective integer program aiming to minimize production costs, time, greenhouse gas emissions, and hazardous waste. They propose and evaluate four evolutionary approaches, including adapted versions of NSGA-II and NSGA-III, to solve this model. The study validates the efficiency of these algorithms using metrics such as hypervolume and spacing. Another study further promotes sustainability by addressing aspects of circularity. Brad and Brad (2021) examine the complexity of designing reconfigurable equipment that satisfies the dual Industry 4.0 requirements of high agility and circular economy compliance. To mitigate the uncertainty in the design process, the authors propose a hybrid evolutionary algorithm combining particle swarm optimization with the theory of inventive problem-solving. This methodology systematically guides designers toward optimal lifecycle concepts, thereby minimizing the design loss function and significantly reducing the number of required iterations.

In summary, while SBO effectively addresses the stochastic and multi-objective nature of RMS, it remains computationally intensive due to the need for iterative, high-fidelity simulations. This bottleneck limits its responsiveness in dynamic settings. To overcome this, research is increasingly turning toward Surrogate Modeling, where learned approximations replace detailed simulations to enable near-instantaneous performance estimation.

2.2 Surrogate Modeling in Manufacturing

In (Misener and Biegler, 2023), two essential conditions for surrogate models applied to process optimization are defined. First, they emphasize the necessity of avoiding overfitting to ensure that the identified optima remain robust to variations in input data. Second, they argue for constraining the search space to the model's validity domain to prevent extrapolation errors and ensure physical feasibility of optimization results. The authors further link these requirements to the stability of optimal solutions through Lipschitz continuity properties. In the same paper, Misener and Biegler (2023) distinguish between surrogate-led and mathematical programming-led approaches. Crucially, they formalize the verification problem to guarantee that surrogate-derived optima align with the true model, validating this framework through industrial case studies. Building on the need for rapid performance evaluation in data-intensive manufacturing systems, recent studies have explored surrogate integration within Digital Twin environments to bridge planning and scheduling. For example, Chua et al. (2021) propose a

Digital Twin-based surrogate using Multivariate Adaptive Regression Splines to estimate production performance from high-dimensional planning parameters, demonstrating accurate prediction of flowtime, tardiness, and utilization in a wafer fabrication case study.

Beyond system-level surrogate modeling, recent work has also advanced surrogate learning at the control and dispatching-rule level. In (Salama et al., 2022), a feature selection framework was introduced to improve the evolvability and compactness of dispatching rules in dynamic job shop environments, demonstrating that informed feature reduction improves both rule quality and learning efficiency. More recently, (Salama et al., 2025) proposed a transformer-based surrogate model for predicting the fitness of dispatching rules in the Flexible Job Shop Scheduling Problem, showing that deep learning surrogates can accurately approximate simulation-based fitness evaluations while achieving significant computational speedups. These results highlight the growing potential of machine learning–driven surrogates as scalable alternatives to exhaustive simulation within scheduling optimization. Complementarily, (Chu and You, 2014) address the computational burden of integrated planning, scheduling, and dynamic optimization in sequential batch processes by embedding surrogate models inside a decomposition-based MINLP framework. Their approach replaces complex linking constraints with surrogate approximations and reduces computational time by several orders of magnitude. Similarly, (Jia et al., 2017) propose a hybrid DES–Kriging framework for demand-driven line availability prediction, confirming the effectiveness of data-driven surrogates in stochastic manufacturing environments.

Providing a comparative perspective on modeling approaches, Papadimitriou et al. (2025) investigate the trade-off between model fidelity and optimization complexity in integrated dynamic scheduling for demand-side management. Using an air separation process as a case study, they compare full-order mechanistic models with various surrogate formulations (linear and nonlinear). Their analysis reveals that while deterministic global optimization with surrogates often faces intractability or infeasibility, stochastic local optimization (multistart) combined with Hammerstein-Wiener surrogate models provides a high-quality data-driven alternative when detailed mechanistic models are unavailable.

While surrogate modeling offers computational efficiency, its integration into holistic and sustainable RMS design remains underexplored. Existing research often isolates objectives like layout and planning, or relies on costly simulations. To enable a unified optimization framework, the next section establishes the system's mathematical foundations in the problem statement and system model.

3. PROBLEM STATEMENT AND SYSTEM MODEL

3.1 Reference RMS Reconfiguration

This study relies on the generic reconfigurable hybrid flowshop model introduced in Bouazza and Kantasa-Ard (2025), where each production stage can dynamically adjust its processing capacity through the addition, removal, or relocation of flexible machine modules. In this framework, reconfiguration consists of modifying the set of active resources at one or several stages in response to forecasted demand variations or shifts in product mix. The model captures both *structural flexibility* (changes in the number and type of machines per stage) and *capacity flexibility* (adapting processing capability over time). As illustrated by the sequence in Fig. 1, the reference system is a three-stage Hybrid Flow Shop. The baseline layout comprises two parallel machines at each stage (M_1–M_2, M_3–M_4, and M_5–M_6). To alleviate bottlenecks, a flexible auxiliary module (M_7) can be assigned to any stage at the beginning of each day. This results in a set of four feasible configurations: the baseline layout and three augmented layouts where M_7 is integrated into any of the stages. In the example depicted, it is initially unused before being added to the second stage, then moved to the third, before being placed at the first stage and finally removed.

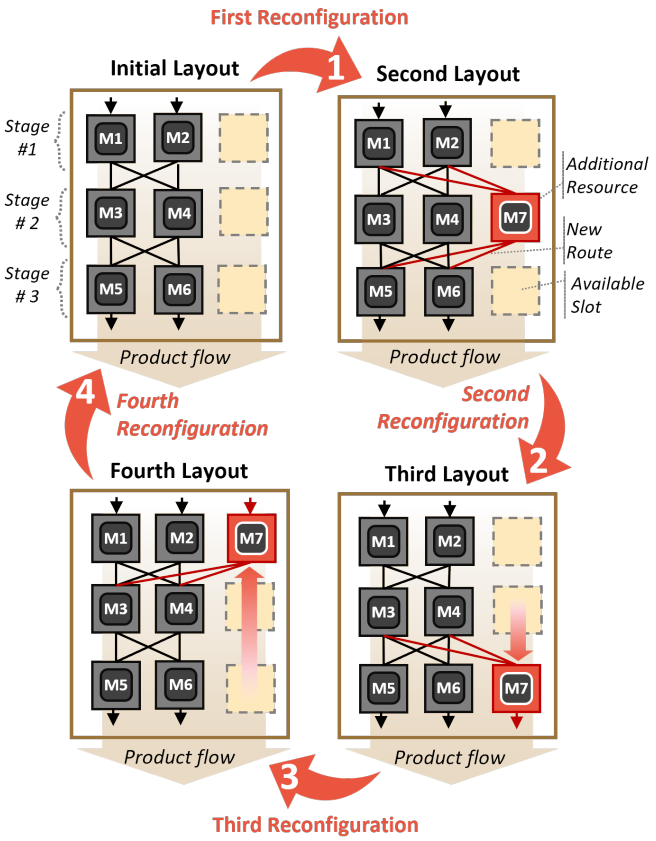


Fig. 1. RMS layout evolution, showing an illustrative reconfiguration sequence across the set of feasible configurations

3.2 Objective Function

Mean Flow Time (MFT) is defined as the average time required for a job to complete all processing stages, measured from its release into the system until its final completion. In addition to MFT, energy consumption is computed following the model proposed by Bouazza and Kantasa-Ard (2025). The Total Energy Consumption (TEC) is obtained by aggregating the energy usage of all workstations, where the consumption of each machine is calculated by multiplying the power rate for each operational state (idle, setup, or processing) by the duration in that state.

The performance of a configuration c under a specific demand scenario s is evaluated using a weighted aggregation of MFT and TEC:

$$F(c,s) = \alpha \cdot \frac{MFT(c,s)}{MFT_{max}} + (1-\alpha) \cdot \frac{TEC(c,s)}{TEC_{max}} \quad (1)$$

where $\alpha = 0.5$ enforces balanced optimization between time-based and energy-based objectives.

The normalization by MFT_{max} and TEC_{max} ensures that both criteria are scaled to the same numerical range, preventing domination of the objective function by metrics with larger absolute magnitudes. This normalization enables fair comparison and consistent weighting between objectives while preserving relative differences.

4. PROPOSED FRAMEWORK

To ensure robust surrogate-model training under realistic demand variability, the proposed framework consists of four main steps: (i) data generation using SBO, (ii) feature engineering, (iii) surrogate model training, and (iv) model testing and validation.

4.1 Data Generation Using SBO

375 demand scenarios across four RMS configurations were simulated using statistically controlled arrival processes. Scenario generation followed bounded distributions for arrival rate, mean inter-arrival time, and arrival timing, ensuring realistic variability in product inflow patterns, including early-arrival skewness and late-arrival clustering effects. For each scenario, a genetic algorithm coupled with a DES model computed three performance indicators for the best configuration: the MFT, the TEC, and a normalized multi-objective fitness value (MFV). Since the first configuration was the best option in only three scenarios, it was removed. To maintain class balance, the remaining scenarios were randomly undersampled so that each configuration was optimal in exactly 124 scenarios. For each scenario, the raw MFT, TEC, and MFV values of the best-performing configuration were retained as regression targets for surrogate model training.

4.2 Feature Engineering

Operation-level simulation outputs were aggregated into scenario-level engineered features to capture the relationships between demand characteristics and system performance. The features describe workload distribution (e.g., total/average operations, variability, and Gini index), arrival-process dynamics (e.g., inter-arrival gaps, arrival ranges, and rates), and product-family composition (e.g., entropy, family proportions, transition frequencies, and run-length statistics). Interaction features further link workload variability with temporal arrival behavior, while temporal-segment descriptors summarize early, mid, and late portions of the scenario horizon. The final dataset comprises 372 scenarios with 51 scenario-level features, the scenario identifier, and three regression targets.

Although the number of features may appear high relative to the dataset size, the features are engineered and aggregated at the scenario level, resulting in a structured representation with low effective dimensionality. In an operational setting, these features can be computed directly from demand forecasts, order release information, and routing/process data, without requiring a prior discrete-event simulation. The DES-SBO process is used only to generate training labels.

4.3 Surrogate Model Training

To construct the surrogate predictors, we evaluated a diverse set of twelve machine learning models, covering linear models, neural networks, and tree-based ensembles. The model set includes Ridge, Lasso, and ElasticNet regressors; a feed-forward MLP; ensemble learners such as Random Forest, Extra Trees, Gradient Boosting, and Histogram Gradient Boosting; and externally optimized gradient-boosting models (XGBoost, LightGBM, CatBoost). In addition, a simple averaging ensemble was implemented to combine the top-performing base models.

All models were trained using the engineered scenario-level features and the three regression targets (MFT, TEC, MFV). Following standard practice, the dataset of 372 scenarios was split using 5-fold nested cross-validation: an outer loop for unbiased performance estimation and an inner loop for hyperparameter optimization via randomized search. Each model was embedded in a preprocessing pipeline, including either robust, standard, or quantile scaling where appropriate. For reproducibility, the hyperparameter tuning procedure was conducted using randomized search with 20 sampled configurations per model, optimized using the negative root mean squared error metric. The inner loop employed 3-fold cross-validation, while the outer loop used 5 folds. A fixed random seed was used across all experiments to ensure consistent results. Linear models were combined with robust scaling, the MLP model used quantile normalization, and tree-based ensemble models were trained without feature scaling. This configuration ensures that both linear and nonlinear models are trained under comparable, controlled, and reproducible conditions. The surrogate model is therefore intended to estimate the best achievable performance under a given scenario, enabling rapid assessment of whether reconfiguration is beneficial without executing the full SBO process.

4.4 Model Testing and Validation

Model validation was conducted exclusively on held-out folds to prevent information leakage. Performance evaluation relied on multiple regression metrics, and inference time was recorded to assess computational efficiency. This design enables a consistent comparison of predictive accuracy and response time across all surrogate models, supporting the identification of fast and reliable predictors suitable for near real-time deployment.

5. EXPERIMENTAL RESULTS

To evaluate the effectiveness of the proposed surrogate modeling framework, three independent regression experiments were conducted to predict the MFT, TEC, and MFV. All experiments followed the same nested five-fold cross-validation protocol, ensuring fair and unbiased performance comparison across models and targets.

5.1 Prediction of Mean Flow Time

As shown in Table 1, linear models (Ridge, ElasticNet, Lasso) achieved near-perfect predictive performance, consistently attaining $R^2 \approx 0.99$. The best-performing results for each evaluation metric are highlighted in **bold** in the table. This indicates that MFT is largely governed by linear relationships with respect to the engineered workload and arrival features, such as operation counts, arrival rates, and workload intensity. The strong performance of regularized linear models further suggests that the feature set captures the dominant structural drivers of flowtime while suppressing noise and multicollinearity effects.

Table 1. MFT Surrogate Model Performance

Model	RMSE	R^2	MAPE (%)	Training time (s)
Ridge	**0.027**	**0.993**	**0.199**	3.579
ElasticNet	0.027	0.993	0.199	1.275
Lasso	0.027	0.993	0.200	**0.326**
AveragingEnsemble	0.040	0.985	0.276	60.923
CatBoost	0.105	0.899	0.696	55.743
GradientBoosting	0.116	0.874	0.807	7.549
XGBoost	0.120	0.865	0.788	13.518
ExtraTrees	0.130	0.845	0.807	7.770
HistGradientBoosting	0.133	0.835	0.915	15.576
LightGBM	0.151	0.789	1.015	28.800
RandomForest	0.176	0.714	1.225	13.185
MLP	0.509	-1.540	3.480	29.202

In contrast, neural networks exhibited poor performance, which can be attributed to the relatively small dataset size and the lack of strong nonlinear relations in the data. As a result, high-capacity models such as MLP tend to overfit the training folds, leading to unstable generalization and degraded validation performance. Similarly, tree-based models showed inferior accuracy compared to linear regression, likely due to their reliance on recursive partitioning, which is less effective when the underlying functional relationships are smooth and globally linear.

5.2 Prediction of Total Energy Consumption

Table 2 shows that TEC prediction is highly accurate across all model families, with several approaches achieving near-perfect or perfect R^2 values. Although RMSE values appear numerically larger, this is primarily a scaling effect caused by the magnitude of energy values rather than model deficiency. This interpretation is further supported by the consistently low MAPE values, corroborating the negligible magnitude of the relative prediction error.

Table 2. TEC Surrogate Model Performance

Model	RMSE	R^2	MAPE (%)	Training time (s)
Ridge	**0.294**	**1.000**	**0.015**	3.651
Lasso	0.507	1.000	0.027	**0.534**
ElasticNet	0.964	1.000	0.051	0.916
AveragingEnsemble	1.618	1.000	0.083	11.757
GradientBoosting	5.089	0.998	0.259	6.655
XGBoost	5.189	0.998	0.270	23.702
ExtraTrees	5.574	0.997	0.285	7.792
HistGradientBoosting	5.557	0.997	0.288	14.688
RandomForest	5.858	0.997	0.300	12.376
CatBoost	6.012	0.997	0.301	55.953
LightGBM	7.486	0.995	0.344	29.822
MLP	46.255	0.815	2.131	44.519

Linear models again demonstrate superior performance, indicating that energy consumption evolves in a largely proportional manner with respect to machine utilization, system workload, and operational duration. Tree-based ensembles provide competitive accuracy but exhibit slightly larger errors, likely due to their piecewise approximation strategy being less effective when modeling smooth monotonic relationships. Neural networks show weaker performance, likely due to their higher capacity relative to the dataset size, resulting in overfitting without meaningful nonlinear patterns to learn.

5.3 Prediction of Multi-Objective Fitness Value

As reported in Table 3, predicting MFV is more challenging than predicting MFT or TEC individually because it combines both objectives into a single globally normalized weighted score, as defined in Eq. (1). The MFV used for regression is not a separate internal GA value; it corresponds to the normalized objective value of the best-performing configuration identified by the GA-DES procedure. This aggregation can compress information and reduce the direct linear structure observed in the individual targets. Among all evaluated models, the Averaging Ensemble achieved the highest predictive accuracy, reaching $R^2 \approx 0.82$ with MAPE values around 12%, but with the longest training time. In contrast, regularized linear regressors delivered nearly identical accuracy with significantly lower overhead, indicating that the composite objective can still be approximated effectively using simpler models.

Table 3. MFV Surrogate Model Performance

Model	RMSE	R^2	MAPE (%)	Training time (s)
AveragingEnsemble	**0.103**	**0.820**	12.032	59.331
Ridge	0.104	0.819	12.032	3.609
Lasso	0.104	0.818	**12.025**	**0.297**
ElasticNet	0.104	0.818	12.172	0.507
CatBoost	0.106	0.811	12.436	54.918
RandomForest	0.107	0.805	12.575	12.245
GradientBoosting	0.108	0.803	12.551	5.789
LightGBM	0.108	0.804	12.655	27.707
XGBoost	0.109	0.800	12.624	12.266
ExtraTrees	0.109	0.800	12.638	8.114
HistGradientBoosting	0.113	0.787	13.397	9.209
MLP	0.169	0.512	18.213	9.602

The underlying linearity of the data, effectively encapsulated by the engineered feature set, is evidenced by the robust performance of the linear models. Ensemble learners provide only marginal improvement beyond this structure, which does not justify their higher training cost. Neural networks again underperform due to the moderate dataset size and weak nonlinear interactions. Overall, these results highlight the trade-off between predictive accuracy and computational efficiency and emphasize that lightweight surrogate models remain preferable for real-time deployment in adaptive RMS decision-support systems.

5.4 Computational Efficiency

Across all experiments, training time was negligible compared with a single simulation-based optimization run, which requires thousands of DES evaluations within a GA loop. Model training ranged from 0.3 s to 61 s, while inference per scenario ranged from 0.003 ms to 0.63 ms, enabling near-instantaneous multi-scenario evaluation for dynamic RMS reconfiguration. In contrast, the reference

SBO process required 2 minutes and 58 seconds per scenario, corresponding to a speedup of approximately five orders of magnitude (10^5) and making performance data immediately available for reconfiguration decisions.

6. CONCLUSION

This paper demonstrated a surrogate modeling approach for RMS optimization using a forecast-driven scenario generation framework. The results showed that Mean Flow Time and Total Energy Consumption are largely linear with respect to the extracted features, allowing regularized linear models to outperform more complex learners. Although the aggregated fitness value was harder to predict due to normalization-related information loss, it remained accurate enough for decision support. The key outcome is a computational speedup of 10^5, replacing costly simulations with rapid, online, energy-aware inference.

From a practical perspective, the proposed methodology separates offline optimization from real-time decision making. SBO is required only during the training stage to generate labeled data, after which the trained surrogate can directly estimate system performance for new demand scenarios. Nevertheless, the approach remains dependent on simulation-generated data, its generalizability to different RMS configurations or unseen demand patterns requires further validation, and the current evaluation is limited to a single case study with a fixed set of configurations.

Future work will focus on extending the framework to heterogeneous topologies, potentially using graph neural networks for layout-agnostic modeling. We also aim to move from prediction to autonomous control by integrating deep reinforcement learning for adaptation to real-time stochastic disturbances.

DECLARATION OF GENERATIVE AI AND AI-ASSISTED TECHNOLOGIES IN THE WRITING PROCESS

The authors used LLMs for language refinement and proofreading, and retain full responsibility for the publication.

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