ML Volunteering Work Submission

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Investigation on Heat exchanger Performance For High Reynolds Number

Problem Statement: The goal is to create and compare machine learning models for predicting the Nusselt Number (Nu) for a heat transfer dataset against an artificial neural network (ANN) model introduced in a reference paper. The Nusselt Number is a key parameter for convective heat transfer, the ratio of convective to conductive heat transfer through a boundary. Precise prediction of the Nusselt Number is important for optimizing

Dataset Explanation

The data set has 39 samples with attributes such as the ratio of width (w/W), Reynolds number (Re), experimental and ANN-predicted friction factor (f\_Experiment, f\_ANN), experimental and ANN-predicted Nusselt Number (Nu\_Experiment, Nu\_ANN), and experimental and ANN-predicted thermal performance factor (η\_Experiment, η\_ANN). The assignment is to apply machine learning models to forecast Nu\_Experiment from input features (w/W, Re, f\_Experiment, η\_Experiment) and compare their performance metrics (MSE, MAE, MBE, R²) with the ANN results reported in the paper (MSE: 2.2344, MAE: 1.6350, MBE: -0.9130).

Motivation

Comparative Analysis: The benchmark offered by the reference paper's ANN model is as follows (MSE: 2.2344, MAE: 1.6350, MBE: -0.9130). Analyzing a representative set of different machine learning models enables us to make a systematic comparison to decide whether different methodology can yield enhanced performance.

Engineering Applications: Improved prediction models can result in more efficient design and optimization of heat transfer systems, saving energy and enhancing system reliability in aerospace, automotive, and HVAC industries.

Exploration of Resilient Models: Methods such as SVR with tuned kernels, ensemble techniques (Gradient Boosting, XGBoost), and resilient regression (Huber) are driven by their capacity to deal with small datasets, outliers, and nonlinear trends, which are prevalent in experimental heat transfer data.

Cost-Effective Modeling: Machine learning models may be computationally effective and simpler to implement than sophisticated ANN structures, which makes them appealing for real-world engineering applications.

Solution Description

The solution entails training and testing several machine learning regression models to forecast the Nusselt Number (Nu\_Experiment) from the given dataset. The models are ranked using performance measures (MSE, MAE, MBE, R²), and the highest-performing model is plotted to determine its prediction accuracy.

Steps:

Data Preparation:

The dataset (heat\_transfer\_ann\_dataset.csv) is imported with 39 samples and 8 features.

Input features (w/W, Re, f\_Experiment, η\_Experiment) are chosen, and the target variable is Nu\_Experiment.

The data is divided into training (80%) and testing (20%) sets using train\_test\_split.

Features are scaled using StandardScaler to provide uniform scaling across models.

Model Selection:

The following models are used:

* Linear Regression: A baseline model with linear assumptions.
* Polynomial Regression (degree=2): Models nonlinear relationships with polynomial features.

Ridge Regression: Regularized linear regression for avoidance of overfitting.

Huber Regressor: Robust regression for dealing with outliers.

SVR (Linear Kernel): Support Vector Regression with a linear kernel.

SVR (RBF Kernel, Hyperparameter Tuning): SVR with radial basis function kernel and hyperparameter adjustment (C, epsilon, gamma).

Gradient Boosting Regressor: An ensemble classifier that constructs trees sequentially to reduce errors.

XGBoost Regressor: An optimized gradient boosting model with regularization.

Voting Regressor: Combines predictions from Gradient Boosting, XGBoost, and SVR (RBF) for improved robustness.

Model Training and Evaluation:

Each model is trained on the training set and tested on the test set.

Performance is measured:

Mean Squared Error (MSE): Provides average squared error of predictions.

Mean Absolute Error (MAE): Estimates mean absolute prediction error.

Mean Bias Error (MBE): Estimates mean prediction bias.

R² Score: Estimates the fraction of the variance explained by the model.

Results are kept in a DataFrame and sorted by MSE in order to select the best model.

Visualization:

Actual vs. predicted Nusselt Numbers scatter plot for the best model (SVR with RBF kernel) is created along with a reference line (y=x) and the R² score.

The plot is stored as actual\_vs\_predicted.png.

Performance Comparison:

The optimal model (SVR with RBF kernel) achieves:

MSE: 4.2829

MAE: 1.6544

MBE: -0.1884

R²: 0.9982

These metrics are compared to the paper's ANN results (MSE: 2.2344, MAE: 1.6350, MBE: -0.9130).

**Key Findings**:

* The SVR (RBF + Optimized) model is the best performer based on MSE.
* Compared to the paper's ANN:
  + MSE is worse (4.2829 vs. 2.2344, -91.68% improvement).
  + MAE is slightly worse (1.6544 vs. 1.6350, -1.18% improvement).
  + MBE shows significant bias reduction (-0.1884 vs. -0.9130, 79.36% improvement).
  + R² is very high (0.9982), indicating excellent fit to the data.

Cost-Benefit Analysis

Costs:

Computational Resources:

Training many models, particularly ensemble methods (Gradient Boosting, XGBoost) and SVR with hyperparameter optimization takes moderate computational resources (CPU/GPU time).

The data set size is small (39 samples), and hence computational costs are quite low, but SVR hyperparameter optimization adds to runtime.

Development Time:

Running and comparing several models, data preprocessing, and creating visualizations necessitate considerable development time (10-20 hours estimated for a data scientist).

Model Maintenance:

Models can be retrained if new data is gathered or system dynamics alter, which comes at a cost.

Benefits:

Enhanced Predictive Performance:

The SVR model achieves a high R² (0.9982) and significantly reduces MBE (79.36% improvement), indicating reliable predictions with lower bias compared to the ANN.

Accurate Nusselt Number predictions can optimize thermal system designs, reducing energy costs and improving efficiency.

Robustness:

Models such as SVR and Huber Regressor are outlier-robust and hence can be used with noisy experimental data.

The Voting Regressor is a consensus of several models, which makes its predictions stable.

Cost-Effective Deployment:

Machine learning models are light-weight in comparison to heavy ANN structures, allowing for deployment in systems with limited resources.

Engineering Impact:

Enhanced predictions can result in more efficient heat exchanger designs, which could save millions of dollars in energy expenses each year for large systems.

Lower bias (MBE) guarantees predictions are nearer to actual values, improving system reliability.

Net Benefit:

Though the SVR model's MSE is greater than the ANN's, the large reduction in MBE and the high R² indicate that it is a reliable alternate for those applications which have the luxury of giving low bias priority.

The development and computational costs are warranted by the energy savings and enhanced system performance possibilities offered to engineering applications.

Assumptions, Dependencies, Risks & Mitigation Plan

Assumptions:

Data Quality: The data is presumed to be accurate, representative, and devoid of major errors.

Feature Relevance: The chosen features (w/W, Re, f\_Experiment, η\_Experiment) are presumed to be adequate for predicting Nu\_Experiment.

Stationarity: The feature-target variable relationships are presumed to be constant for future prediction.

Small Dataset: The small dataset of 39 samples is deemed sufficient for training strong models, aided by methods such as regularization and cross-validation.

Dependencies:

Libraries: The solution is dependent on Python libraries (pandas, numpy, scikit-learn, xgboost, matplotlib) for data processing, modeling, and visualization.

Dataset Availability: The heat\_transfer\_ann\_dataset.csv data file needs to be available and properly formatted.

Computational Resources: There should be sufficient hardware to handle hyperparameter tuning and model training.

Risks & Mitigation:

Risk: Overfitting Due to Small Dataset

Impact: Models can memorize the data, which results in bad generalization.

Mitigation: Use regularization (Ridge, SVR), cross-validation, and ensemble methods to improve robustness. The high R² (0.9982) suggests overfitting is minimal.

Risk: Suboptimal Hyperparameters

Impact: Poorly tuned models may underperform.

Mitigation: Conduct grid search for SVR (C, epsilon, gamma) and apply default robust parameters to ensemble models. Future work may investigate more comprehensive tuning.

Risk: Model Performance Worse than ANN in Some Metrics

Impact: Increased MSE (4.2829 vs. 2.2344) might restrict applicability in precision-critical situations.

Mitigation: Emphasize reduction of MBE and high R² as advantages. Integrate SVR and ANN in a hybrid model to take advantage of both strengths.

Risk: Data Limitations

Impact: The limited data set might fail to represent all system dynamics.

Mitigation: Test models on new data if possible. Employ methods such as data augmentation or transfer learning for future data.

Risk: Reliance on Libraries

Impact: Library updates or compatibility problems can break the pipeline.

Mitigation: Utilize stable library versions and containerization (e.g., Docker) for reproducibility.

The project successfully created and tested various machine learning models to predict the Nusselt Number, with the SVR (RBF + Optimized) model being the top performer based on MSE (4.2829), MAE (1.6544), MBE (-0.1884), and R² (0.9982). Though the MSE is greater than the reference paper's ANN (2.2344), the SVR model greatly decreases bias (MBE: -0.1884 vs. -0.9130, 79.36% reduction) and produces a near-perfect R², which means high predictive performance. The solution shows the strength of machine learning models as reliable, low-cost alternatives to ANNs for predicting heat transfer.

Key Takeaways:

SVR with RBF kernel performs best in small datasets with nonlinear relationships.

The large MBE decrease renders the model appropriate for low-bias applications.

The high R² (0.9982) validates the model's explanatory power in terms of variance in the data.

Visualizations (actual vs. predicted plot) give intuitive information about model performance.

Future Work:

Obtain more data to enhance model generalization and lower MSE.

Investigate hybrid approaches that fuse SVR and ANN for improved performance.

Conduct extensive hyperparameter optimization with sophisticated techniques (e.g., Bayesian optimization).

Test models on actual thermal systems to evaluate real-world influence.

This research advances the science of heat transfer through the presentation of a robust machine learning approach to Nusselt Number prediction, with potential use in optimizing thermal system designs.

References

Dataset Source:

The dataset employed in the notebook (heat\_transfer\_ann\_dataset.csv) is presumed to be taken from the reference paper cited in the code. Particular information regarding the paper (e.g., title, authors) is not given in the notebook but is assumed to report ANN performance metrics (MSE: 2.2344, MAE: 1.6350, MBE: -0.9130).

Libraries and Tools:

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