19th Brazilian Congress of Thermal Sciences and Engineering
November 6th–10th, 2022, Bento Gonçalves - RS - Brazil

ENCIT2022-0135
Evaluation of Machine Learning models to predict the thermal performance of Active Magnetic Regenerators

Marco Antônio Cerutti de Lima
marco.lima@polo.ufsc.br
Guilherme Fidelis Peixer
guilherme.peixer@polo.ufsc.br
Jaime Andrés Lozano Cadena
jaime@polo.ufsc.br
Jader Riso Barbosa Jr.
jrb@polo.ufsc.br

POLO – Research Laboratories for Emerging Technologies in Cooling and Thermophysics, Department of Mechanical Engineering, Federal University of Santa Catarina, Florianópolis, SC, 88040-900, Brazil

Abstract. *Machine Learning (ML) and data-driven modeling has developed drastically over the past years. Novel applications are tested constantly, thriving when fast and accurate predictions with high modeling complexity are involved. Active Magnetic Regenerators (AMR), the heart of magnetic refrigerators, are an example of such scenarios. The modeling of these components involves non-linear equations for thermal, hydraulic and magnetic domains, closure relations, material properties and application of numerical methods. However, numerical solutions are hindered in applications where many simulations, such as optimization problems, or for fast predictions, such as predictive control, are required. Despite that, AMR modeling through ML is not well established in the literature. This work seeks to explore different ML techniques in the prediction of the performance of AMRs. The evaluated techniques were Linear Regression; Ridge Regression with Second, Third and Forth degree Polynomial Features; Random Forest; K-Nearest Neighbours; Support Vector Regression; Extreme Gradient Boosting and Neural Networks. The models were evaluated by the test set coefficient of determination (R^2). The best results were given by the Ridge Regression with Third degree Polynomial Features and Neural Network, with R2 of 0.998 and 0.993, respectively.*

Keywords: *Magnetic Refrigeration, Machine Learning, Active Magnetic Regenerators*

1. INTRODUCTION

Refrigeration systems are fundamental elements of a large share of modern society, providing thermal comfort, food storage and a wide range of temperature control in processes and devices. The majority of the systems employed, especially the ones focused on household applications, rely on a combination of vapor compression and expansion and phase change heat transfer. However, the search for alternative technologies has gained traction over the last decades with the phase-out and phase-down of refrigerant fluids agreed internationally on the Montreal Protocol, and more recently on the Kigali amendment.

Among the many alternatives under evaluation, magnetocaloric systems are considered as the most promising of the so called not-in-kind cooling technologies. The technology, which is based on the magnetocaloric effect, employs solid materials as refrigerants, hindering the possibility of leakages and reducing the environmental impact. Moreover, the magnetocaloric effect is reversible for many of the benchmark alloys employed in magnetocaloric refrigerators, which has the potential to enable the systems to operate, theoretically, at high efficiencies. Despite that, several challenges are still posed to magnetocaloric refrigeration systems preventing its commercial application and operation at high efficiencies. Amongst the most prominent challenges, one can highlight the complex modeling of the components of magnetocaloric systems, particularly the Active Magnetic Regenerator (AMR). Such process involves the solution of the momentum and energy conservation equations, usually via numerical methods such as Finite Volumes, complex thermo-magnetic characterization and a delicate coupling between hydraulic and magnetic profiles. All of that entails computationally costly simulations, which is critical for optimization analysis where hundreds of thousands of simulations may be required, preventing the achievement of optimal configurations of magnetic refrigeration systems.

For such challenges, data-driven modeling and ML techniques are being applied in a wide range of engineering problems. These methods rely on the fitting of statistical correlations among the design variables and the performance metrics of a problem, commonly denominated as learning. The models can be computationally costly to train, but are eventually able to provide fast and accurate predictions of performance metrics, ideal for optimization of thermal systems.

Kwon *et al.* (2020) explored ML techniques for the regression of heat transfer coefficients.The authors employed the Random Forests (RF) algorithm to predict convection heat transfer coefficients, achieving a coefficient of determination (R^2) of 0.966. Similarly, Montanez-Barrera *et al.* (2022) presents a Artificial Neural Networks (ANN) technique to predict the pressure drop of zeotropic mixtures in micro-channels. The authors applied a methodology known as Transfer Learning, enhancing the models results by providing the pressure drop from an empirical correlation as a feature, improving performance and generalization capabilities of the network.

Regarding the modeling of refrigeration systems, Ertunc and Hosoz (2006) employed ANN to predict the performance of a refrigerator with an evaporative condenser. The authors used the network for calculating the heat rejection rate, refrigerant mass flow rate, compressor power, and coefficient of performance. Likewise, Ledesma and Belman-Flores (2016) presented the application of an ANN to predict the Coefficient of Performance of a vapor compression refrigeration system. The authors developed an optimization processes, seeking to identify the design parameters with the largest impact on the coefficient of performance. Maiorino *et al.* (2022) proposed a novel predictive control methodology based on the use of ANN to optimize the delay between the cycles of operation of an on-off fixed speed compressor in a vapor compression refrigeration system.

When it comes to magnetocaloric refrigeration systems, there are few works in the literature focused on the application of ML techniques. Aprea *et al.* (2017) developed a control technique based on ANN to optimize the operation of a rotary permanent magnet magnetic refrigerator. Silva *et al.* (2020) compared 4 different ML methods for the prediction of magnetocaloric heat pumps temperature span, heating power and coefficient of performance. The evaluated models were the Ordinary Least Squares, Ridge Regression, Lasso Regression and K-Nearest Neighbors. Maiorino *et al.* (2021) proposed a numerical model based on ANN to calculate the thermo-magnetic properties of magnetocaloric materials, allowing their implementation in numerical models of AMRs. The use of ANN to integrate the properties of magnetocaloric materials into AMR models was compared against the more commonly used Curie Temperature Shift Method, reducing the temperature error from 13 K to 6.6 K for a seven-layer configuration and from 4.1 K to 1 K for a four-layer configuration.

Given the few works focused in applications of ML techniques in AMRs, and the lack of a comparison of different methods, the main objective of this work is to develop ML models capable of predicting the cooling capacity ($\dot{Q}_{\mathrm{C}}$) of AMRs using data from numerical models. This work also aims to evaluate the performance of each method, compare them using a quality metric and graphical analysis, and select the ones with the best results for further study. Moreover, some ML techniques which were used in this work present the capability of easily order the design parameters which incur the most variance in the predicted results. This means that the design variables used in training can be sorted by relative importance in the overall performance metric under evaluation. As such, a secondary objective of this works is to evaluate, whenever possible, the relative importance of each variable in determining simulations results of cooling capacity.

2. METHODOLOGY

The training phase of ML models requires the supply of adequate data for the algorithm to learn. This data must be accurate and representative of the process or phenomena under evaluation, being the quality of the input data a fundamental aspect for the success of the model development. The database used in this work is composed of 533 simulations from a numerical model (Vieira *et al.*, 2021) aiming for the design of a magnetic air conditioning system with a cooling capacity of 2600 kW (9000 Btu/h). As mentioned above, the database contains only numerical data, with the following input parameters: AMR height (H), width (W) and length (L), applied magnetic flux density (B), liquid mass flow rate ($\dot{m}_{\mathrm{f}}$), frequency of operation (f), and fluid inlet temperatures at the cold (T_{C}) and hot (T_{H}) ends of the AMR. The range of each design variable is determined on the authors' knowledge of the air conditioner operating conditions (Peixer, 2020). The range of the design parameters is presented in Table 1.

Table 1: Range of the design variables utilized as features for the Ml models

Parameter [unit]	Min	Max
W [mm]	45	70
H [mm]	28	55
L [mm]	120	160
B [T]	0.8	1.5
$\dot{m}_f$ [kg/h]	350	850
f [Hz]	0.5	4
T_C [°C]	14	19
T_H [°C]	39	44

2.1 Machine Learning Framework

In order to investigate the viability of using a ML approach to AMR simulations, 7 different ML models were tested: Linear Regression , Ridge Regression with N-Polynomial Features, Random Forest (RF), K-Nearest Neighbours (KNN), Support Vector Regression (SVR), Extreme Gradient Boosting (XGBoost) and Artificial Neural Networks (ANN). The models were implemented in the Python programming language, using the open source ML library Scikit-Learn (Pedregosa *et al.*, 2011), with the exception of the ANN, which was implemented with the Keras (Chollet *et al.*, 2015) framework with a Tensorflow (Abadi *et al.*, 2015) backend. The employed models were:

- **Linear Regression (Press *et al.*, 2007):** The most common and simple regression method. Assumes that the input and output variables follow linear patterns and works by minimizing the standard deviation between ground target data and the predicted values;

- **Ridge Regression with N-Polynomial Features (Hoerl and Kennard, 1970):** Consists of a combination of the Ridge regression technique, used as a regularization method, and the combination of the input parameters up to n^{th} order, seeking to incorporate non-linear patterns in the equation.

- **Random Forest (Ho, 1995):** Consists of a technique called bagging to build full decision trees in parallel from random bootstrap samples of the data set. The final prediction is an average of all of the decision tree predictions. Random forest "bagging" minimizes the variance and overfitting. Different hyperparameters for the algorithm were optimized, including the number of decision trees, and depth of tree;

- **K-Nearest Neighbors (KNN) (Cover and Hart, 1967):** Evaluates the distance between parameters of each data point on a hyperplane, and makes predictions based on the K data points closest to the object. Different hyperparameters for the forests were optimized, such as the value of K and the distance metric.

- **Support Vector Regression (SVR) (Cortes and Vapnik, 1995):** Determines a hyperplane that minimizes the error between the target data and the predicted values, allowing errors within an established margin to not be taken into account. Different hyperparameters for the algorithm were optimized, including the regularization, and the magnitude of the error margin;

- **Extreme Gradient Boosting (XGBoost) (Chen and Guestrin, 2016):** A decision tree ensemble learning algorithm similar to RF, wherein the process of additively generating weak models is formalized as a gradient descent algorithm over an objective function. Gradient boosting sets targeted outcomes for the next model in an effort to minimize errors, which are based on the gradient of the error with respect to the prediction. Different hyperparameters for the algorithm were optimized, including the learning rate, and number and depth of trees;

- **Artificial Neural Network (ANN) (McCulloch and Pitts, 1943):** Artificial NNs use a concept known as perceptron, which works receiving inputs from a finite amount of features. Each feature is multiplied by a weight, which are then all summed together. The total sum is then input to an activation functions that determines final output of the layer. Different hyperparameters for the algorithm were optimized, including the number of layers, number of neurons in each layer and activation function for each layer.

In order to systematically attest the quality of each ML approach in predicting $\dot{Q}_{\mathrm{C}}$, the database was separated in 2 groups: training and test sets. The training set contained data used to fit the models, and was further divided into two distinct groups: an actual train set and a second group know as validation set. The train set was employed to enable each one of the algorithms to learn, while the validation set was utilized to asses the results of each model when cross validation was employed.

Validation in ML is a fundamental step to guarantee that the models do not have significant bias towards the training data. When it occurs, it is said that the model is overfitting. (which happened to one the models present in this work, as will be shown in the following sections). An approach to prevent that, besides the specific hyperparameter tuning for each model, is the so called Cross-validation. Cross-validation takes a fixed number of partitions (also known as "folds"), employs all but one of the folds as training data while the remaining fold is used as validation set. The models are trained until each the folds is used as test set. Then, the model averages the overall predictions of all folds and creates the final model.

Some parameters of a ML model, must be provided to the model before the training phase, being called Hyperparameters. Optimal values for Hyperparameters are, *a priori*, unknown, and must be evaluated by some sort of algorithm. Methods for testing Hyperparameters have been developed and integrated into both the Scikit-Learn (Pedregosa *et al.*, 2011) and Keras (Chollet *et al.*, 2015) libraries and used in this work. The most simple of these is Grid Search, a brute force approach which tests all possible combinations from a given matrix of values (LaValle *et al.*, 2004). This algorithm was used for RF, KNN, SVR and XGBoost models. For ANN, Hyperband (Li *et al.*, 2016) was used instead. Lastly, the performance of the models was quantified in terms the coefficient of determination (R^2).

3. RESULTS

3.1 Graphical Analysis of Models

This section presents the results of the trained models in a graphical manner, where the ground truth for the cooling capacity are plotted in the x-axis and the predicted outcomes in the y-axis. To aid the visualization plus and minus 10 % error bars are presented in each plot. The results are presented for both the training and test sets. The results for the Linear regression and Ridge Regression with Second, Third and Forth degree polynomial features are presented in Figure. 1.

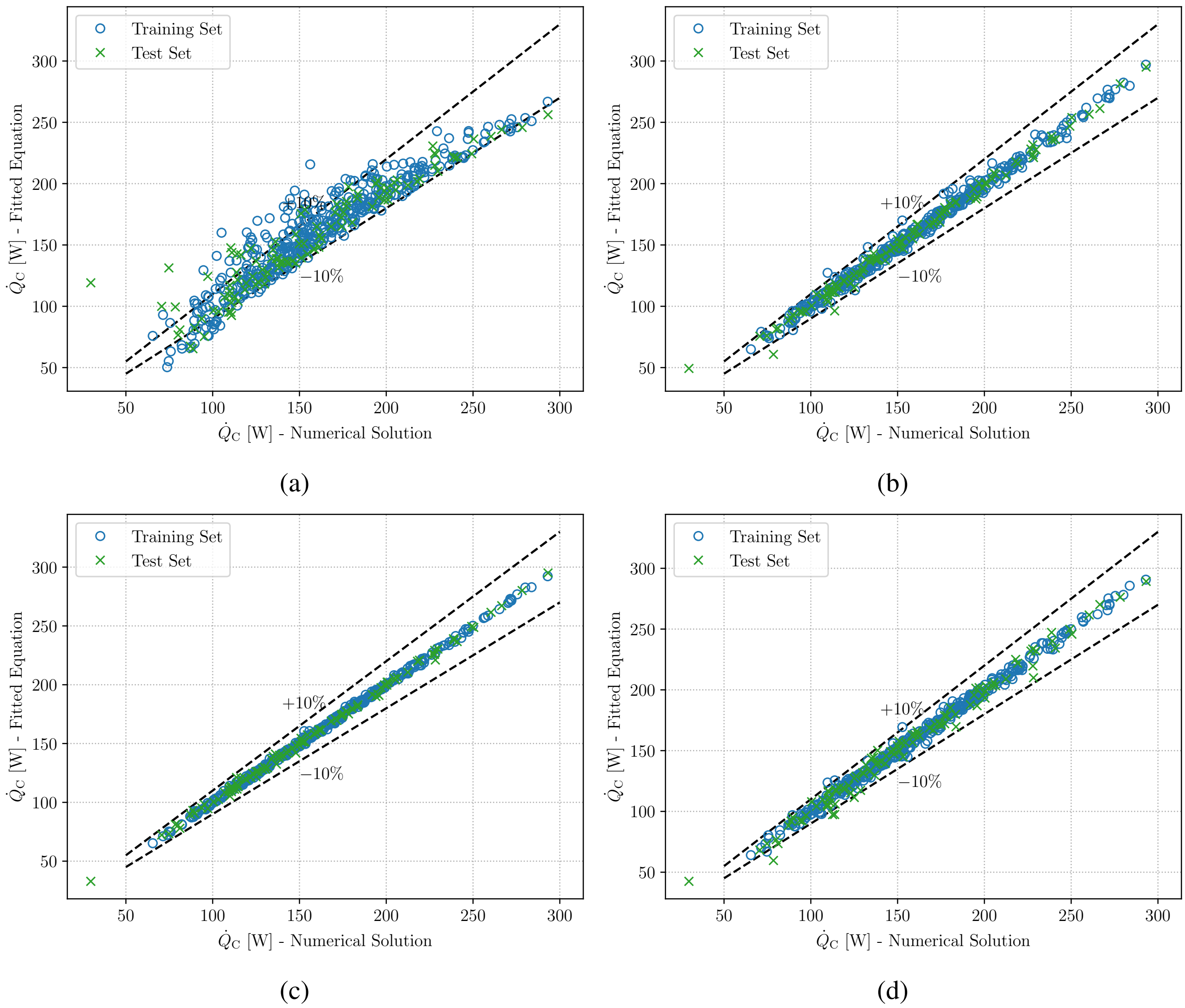


Figure 1: Comparison between the ground truth cooling capacity and the predicted outcomes. The figures depict the results for (a) Linear regression, (b) Ridge regression with second-degree polynomial features, (c) Ridge regression with third-degree polynomial features and (d) Ridge regression with forth-degree polynomial features.

According to Figure. 1 (a) the Linear Regression could not properly predict the target values of the AMR cooling capacity, and a non-linear trend can be observed in the plots of the predicted outcomes. This result was somewhat expected and is linked to the highly non-linear phenomena involved in the operation of AMRs, *e.g.*, heat transfer and thermal magnetic coupling. When the Polynomial Features technique is used to transform the features, one can observe from Figures 1(b)-(d) that the model accuracy and precision are greatly improved, given that non-linear effects can now be incorporated into the model. The best correlation was provided by the Third-Degree Polynomial features, given that higher order polynomials start to destabilize the model. The Ridge Regression was utilized with a ridge coefficient of 0.5 and was able to prevent overfitting the model. The results for KNN, RF, SCR and XGBoost are presented in Fig. 2.

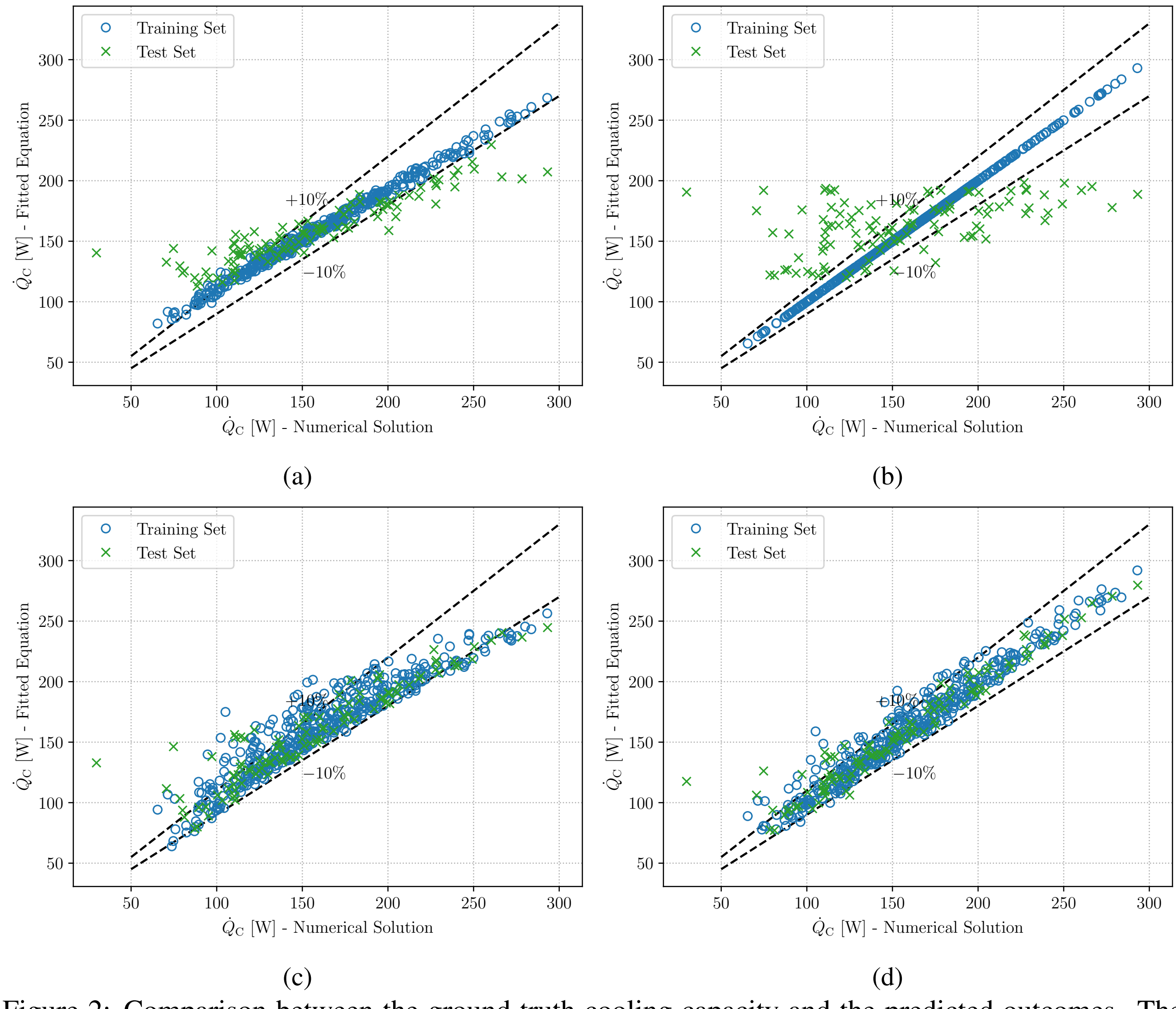


Figure 2: Comparison between the ground truth cooling capacity and the predicted outcomes. The figures depict the results for (a) RF, (b) KNN, (c) SVR and (d) XGBoost.

Figure 2(a) demonstrates that the predictions provided by the RF model are not linearly aligned with the ground truth values, showing a slight overfitting tendency. On the other hand, Figure 2(b) demonstrates that the KNN model severely overfits to the numerical data. Although the model was able to predict with a 100 % accuracy the results for the training set, it failed to the same in the test set, and also presented the worst result of all models evaluated in the present work. Figure 2(c) shows that the SVR model has presented a similar trend to the Linear Regression, although the incorporation of an error margin and non-linear kernels enable the model to better predict the target values. Additionaly, the results for the XGBoost model depicted in Figure 2(d) demonstrate that is was able to predict the results accurately, but with low precision. That can be noted by the scattering around the error lines. Lastly, the results for the ANN are presented in Figure 3.

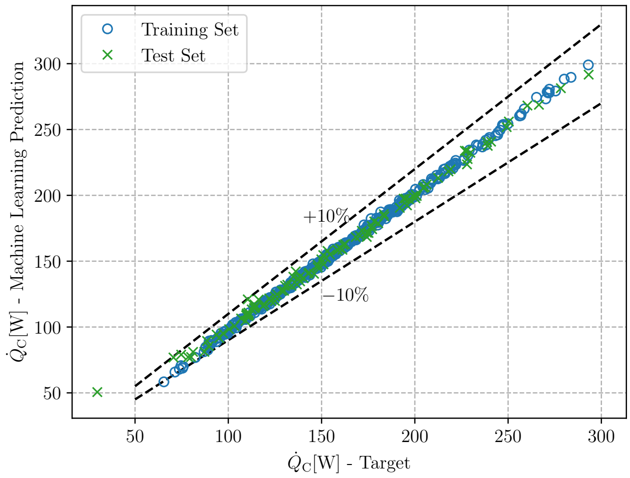
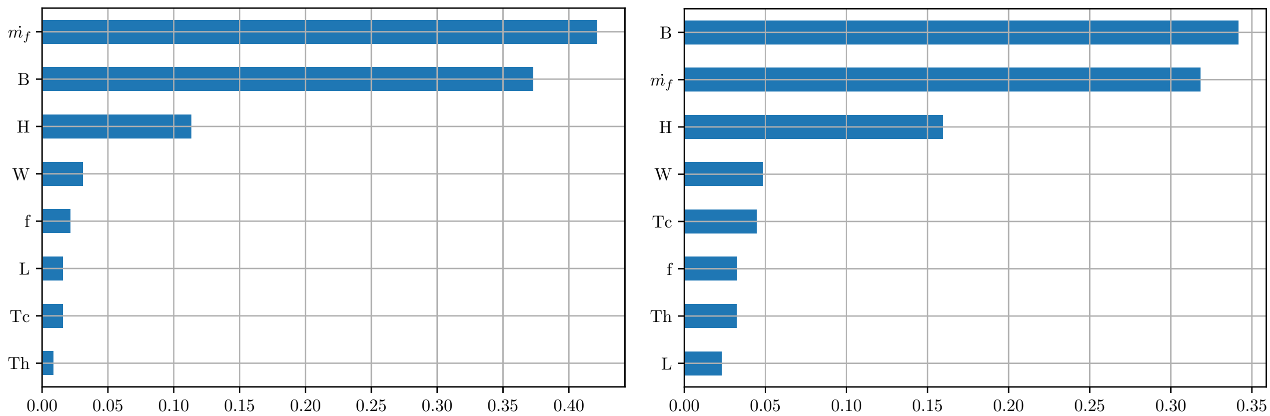


Figure 3: Comparison between the ground truth cooling capacity and the predicted outcomes for the ANN.

As expected, the ANN was able to predict with high accuracy and precision the performance of AMRs, as depicted in Figure 3, ranking among the best results obtained in this study. Besides that, the model was the one which demanded the highest computational power for its training.

3.2 Feature Importance

Among the models evaluated, the ones based on decision trees provide a ranking of the importance of the input variables on the model results. This way, RF and XGBoost allow for the extraction of the relative importance of the input parameters, shown in Fig. 4.



(a) Random Forest (b) XGBoost

Figure 4: Relative importance of the input variables obtained with (a) RF and (b) XGBoost.

Even though the results shown in Figure 4 have some discrepancies, it is worth mentioning that both models attributed the highest importance for the mass flow rate and magnetic flux density, which are in agreement with optimization results generated by Peixer (2020). Moreover, the height and width of the AMR appear as the next most important parameters on the list, reinforcing the importance of

AMR geometry on its performance. The low importance obtained by the inlet temperatures, both at the hot and cold side, is attributed to their limited variation in the design space, whereas the ones by the frequency and length attributed to larger effects generate by similar features, *i.e.*, the mass flow rate being an operational feature with higher importance than the frequency, and the height a dimensional feature of the AMR with higher importance than its length.

3.3 Model Accuracy: Coefficient of Determination

Complementing the graphical evaluation carried out previously, a quantitative evaluation of the models is performed through the coefficient of determination as shown in Table 2.

Table 2: Coeficient of Determination for all the models trained in this work

Model	R^2
Linear Regression	0.8861
Ridge Regression with 2nd Degree Polynomial Features	0.9925
Ridge Regression with 3rd Degree Polynomial Features	0.9980
Ridge Regression with 4th Degree Polynomial Features	0.9867
Random Forest	0.6701
K-nearest Neighbors	0.2093
Support Vector Regressor	0.8381
Extreme Gradient Boost	0.9331
Artificial Neural Network	0.9930

It is clear from Table 2 that the conclusions obtained qualitatively by the graphical analysis are in accordance with the ones obtained quantitatively by the coefficient of determination. The models with the best accuracy were the Ridge Regression with Third-Degree Polynomial Features and the Artificial Neural Network, and the worst model was the KNN.

4. Conclusions

This work evaluated the capability of 9 ML techniques in the prediction of the cooling capacity of AMRs for magnetic refrigeration. The performance of the models were evaluated qualitatively, by graphical analysis, and quantitatively, by the coefficient of determination. The results demonstrated that the best models were the Third-Degree Polynomial Features and the Artificial Neural Network, and the worst model was the KNN. When computational power for the training of the models is not an issue, the authors recommend the use of ANN due to its lower susceptibility of overfitting when compared to the Ridge Regression with Third-Degree Polynomial Features. If computational power is an issue, the Ridge Regression with Third-Degree Polynomial Features can be trained with fast and does not require cross validation nor hyperparameter tuning techniques.

5. ACKNOWLEDGEMENTS

Financial support from CNPq, CAPES, CODEMGE and the EMBRAPII Unit Polo/UFSC is duly acknowledged.

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