Towards Accurate Size Predictions of Magnetic Nanoparticles Using Support Vector Regression

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This study explores the size of magnetic nanoparticles (MNP) for applications in Magnetic Resonance Imaging (MRI) and Magnetic Particle Imaging (MPI). Emphasizing the critical role of MNP size on their response to alternating magnetic fields, the study unveils a regression model to optimize MNP synthesis towards tailored sizes of MNP. With a limited and broadly distributed data set at hand, the feasibility of building an accurate predictive model based on Support Vector Machines is shown. Integrating such a model into a continuous synthesis setup establishes a feedback loop, enabling real-time control and adaptation of synthesis parameters.

Keywords:
magnetic nanoparticles
synthesis,
machine learning,
Support Vector Machines,
size prediction,
process optimization

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I Introduction

Magnetic nanoparticles (MNP) have emerged as pivotal entities in the area of medical technology, offering unique advantages in diagnostic and therapeutic applications [1, 2]. This study delves into the optimization of MNP synthesis, with a particular focus on MNP size, to enhance their performance in alternating magnetic fields — an essential consideration for applications in Magnetic Resonance Imaging (MRI) and Magnetic Particle Imaging (MPI) [3]. The complex nonlinear behaviour of MNP in alternating fields [4, 5] underscores the critical role of MNP size, making it a focal point of investigation in this research.

Further, utilizing MNP holds tremendous potential in revolutionizing medical treatments, especially in the context of hyperthermia [6, 7]. Thus, the need for fine-tuned control over MNP characteristics becomes paramount. Achieving optimal magnetic response in alternating fields is crucial for unlocking the full potential of MNP in hyperthermic applications, where precise and targeted heating is essential for therapeutic efficacy.

The aim of this comparative study is to find a regression model that can accurately predict the size of MNP based on the system parameters of their continuous synthesis process. By incorporating regression models into the continuous automated synthesis setup, a sophisticated feedback loop is envisioned, creating a dynamic system that seamlessly adapts synthesis parameters based on real-time data.

II Material and methods

This study explores regression models for predicting MNP size in a comparative analysis. The data is taken form an experimental study of a continuous MNP synthesis that has been already published [8]. The dataset includes all system parameters of the synthesis setup, educt concentrations and measured MNP sizes.

The data comprises of 26 data points, each representing a single synthesis run. Each data point contains 22 features and the MNP size as the target variable.

The preparation of the data set includes the handling of missing values by either zero or mean imputation for different types of features. Data normalization and One-Hot-Encoding are applied as a last data preprocessing step to ensure an effective and unbiased modelling of the relevant features.

For the size prediction, a Support Vector Regression (SVR) [9] model was built and compared to an Elastic Net Regression [10], a regularized linear regression algorithm.

An extensive grid search was designed to find the best hyperparameters for each regression method. To account for the limited number of data points within the two data sets, an extensive cross-validation was employed. Leave-One-Out-Cross-Validation uses each single data point as a validator against the remaining data points during training, to minimize the training bias and allow a reliable performance estimation [11]. With the optimized hyperparameters for each method, the final prediction was performed with a random data split where 80 % of the data points were used as training set and the remaining 20 % constituting the validation set.

During the grid search and the final training of the models, the Root-Mean-Squared-Error (RMSE) function was used as evaluation metric. RMSE was chosen to ensure precise MNP size estimation due to its high sensitivity towards large errors.

III Results and discussion

Table 1 shows both examined regression methods and their determined hyperparameters. All hyperparameters are determined by comprehensive testing within reasonable intervals to ensure thorough exploration of the model's parameter space.

The alpha hyperparameter in Elastic Net controls the overall strength of regularization, with a value of 0.532 emphasizing a moderate regularization effect, which helps to prevent overfitting. The L1-ratio determines the balance between L1 and L2 regularization, with a value of 0.1 indicating a strong preference for L2 regularization, which is suitable to avoid feature selection.

For SVR, the optimal C value at 152.59 shows low regularization implying adaptability to specific data points. Gamma influences the shape of the regression curve. A value of 3.16 indicates sensitivity to local variations. A small epsilon of 0.1 means that the model is less tolerant to deviations in the predictions, which goes along with the desired accuracy in the MNP size prediction. The selected Radial Basis Function (RBF) kernel allows the model to capture complex relationships.

Figure 1 shows a bar chart with the RMSE values and the standard deviation of the residuals for each tested method with its identified hyperparameters.

The Elastic Net model yielded an RMSE score of 40.2, and thus has a high average magnitude of prediction errors resulting in less accurate predictions. Additionally, the standard deviation of residuals for Elastic Net is 104.57, signifying substantial variability in the prediction errors around the regression line.

Table 1: Determined hyperparameters

Method	Hyperparameter	Tested Ranges	Best Value
Elastic Net	alpha L1-ratio	[0.0, 1.0] [0.1, 1.0]	0.532 0.1
Support Vectors	C gamma epsilon kernel	[100.0, 200.0] [0.0, 5.0] [0.1, 1.0] ['linear', 'poly', 'sigmoid', 'rbf']	152.59 3.16 0.1 rbf

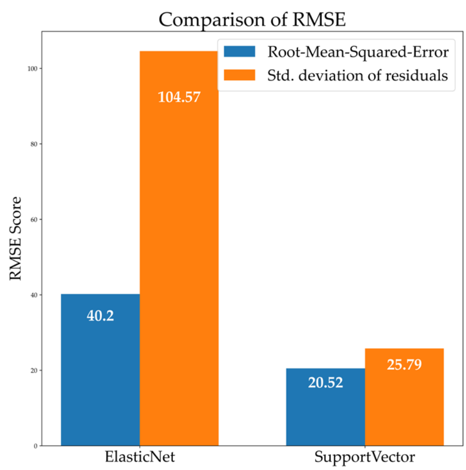

Figure 1: Validation scores for the trained regression methods with their RMSE score (blue) and the standard deviation of the residuals (orange).

In contrast, the Support Vector Regression model performed better with an RMSE score of 20.52, indicating lower prediction errors. The narrower standard deviation of residuals 25.79 in Support Vector Regression implies that it captures the underlying patterns more effectively.

Overall, the data suggests that Support Vector Regression is more suitable to accurately predict sizes of MNP. The underlying synthesis involves complex non-linear feature correlations, which can be captured via the radial basis function. For their applications, a tailored MNP size is significant. A fine tuning of the hyperparameter epsilon can prioritize accurate predictions and still allow a small error margin to enhance robustness. By definition of SVR, outliers (exhibited by experimental variability or measurement errors), are not considered.

However, given the small dataset size, high feature dimensionality, and broad distribution of MNP sizes, specific model selection and validation are crucial. Further cross-validation and exploration of domain-specific feature engineering and consideration of additional types of regression methods can enhance the robustness of the predictions.

IV Conclusion and outlook

In this study, two regression methods were assessed and compared towards their suitability regarding an accurate MNP size prediction. The two methods, Elastic Net Regression and Support Vector Regression, were investigated using a small data set of different synthesis and compared using an error function (RMSE) and the standard deviation of the prediciton residuals. The study shows, that the Support Vector Regressions yields a much smaller RMSE value of 20.52 compared to 40.2. Also its standard deviation is smaller with 25.79 compared to 104.57, which indicates a smaller variation within the prediction errors. Both values indicate an accurate precision and the suitability of the employed SVR. However, as only limited and broadly distributed data was available for comparing the two methods, an extended study incorporating a larger dataset is necessary to validate the findings. Also, the performance of other regression methods such as random forests, gradient boosting or multilayer perceptrons should be considered and compared to the ones presented in this work.

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