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Boosting-based model for solving Sm-Co alloy's maximum energy product prediction task

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ABSTRACT

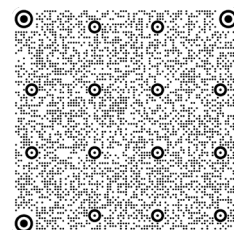
Purpose: This paper aims to decide the Sm-Co alloy's maximum energy product prediction task based on the boosting strategy of the ensemble of machine learning methods.

Design/methodology/approach: This paper examines an ensemble-based approach to solving Sm-Co alloy's maximum energy product prediction task. Because classical machine learning methods sometimes do not supply acceptable precision when solving the regression problem, the authors investigated the boosting ML model, namely Gradient Boosting. Building a boosting model based on several weak submodels, each of which considers the errors of the prior ones, provides substantial growth in the accuracy of the problem-solving. The obtained result is confirmed using an actual data set collected by the authors.

Findings: This work demonstrates the high efficiency of applying the ensemble strategy of machine learning to the applied problem of materials science. The experiments determined the highest accuracy of solving the forecast task for the maximum energy product of Sm-Co alloy formed on the boosting model of machine learning in comparison with classical methods of machine learning.

Research limitations/implications: The boosting strategy of machine learning, in comparison with single algorithms of machine learning, requires much more computational and time resources to implement the learning process of the model.

Practical implications: This work demonstrated the possibility of effectively solving Sm-Co alloy's maximum energy product prediction task using machine learning. The studied boosting model of machine learning for solving the problem provides high accuracy of prediction, which



reveals several advantages of their use in solving issues applied to computational material science. Furthermore, using the Orange modelling environment provides a simple and intuitive interface for using the researched methods. The proposed approach to the forecast significantly reduces the time and resource costs associated with studying expensive rare earth metals (REM)-based ferromagnetic materials.

Originality/value: The authors have collected and formed a set of data on predicting the maximum energy product of the Sm-Co alloy. We used machine learning tools to solve the task. As a result, the most increased forecasting precision based on the boosting model is demonstrated compared to classical machine learning methods.

Keywords: Sm-Co alloys, Ensemble learning, Gradient boosting, Small data, Prediction accuracy

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METHODOLOGY OF RESEARCH, ANALYSIS AND MODELLING

1. Introduction

For the last few decades, the progress in material science has been associated with such paradigms as "computational science", "big data", "material informatics", and "data-driven". Reviews [1-4] describe in an excellent way the historical aspects and leading features of the development of the machine learning (ML) approach for solutions to material science problems. It is evident that experimental research in materials science takes a long time and requires significant resources and expensive equipment. For instance, finding new materials takes 10 to 20 years from study to the first usage [5]. At the same time, Material Genome Initiative (MGI) [6] considers ML-based methods as a tool for discovering, developing, and improving modern materials twice as fast with a significant cost reduction. Due to MGI and open access resources like NOMAD [7], Materials Project [8], Aflowlib [9], and OQMD [10], the rapidly growing of works in this area has taken place for the last years [1,2]. The various types of research involve predicting materials properties [11-13], discovering new compounds [14], modelling professional risk [15], solving the problems of classification [16,17], regression [18,19] and clustering [20], searching the hidden relationships [21], etc.

However, along with the apparent advantages, machine learning methods in materials science have characteristics that complicate the search, collection, analysis, and application for practical purposes of the necessary data. Firstly, the past data obtained by experiments or simulations must be available. The challenges are that data from diverse sources, as a rule, are presented differently (text, tables, figures), contain unspecified dependencies, and property values are sometimes given in different measurement units.

In addition, they often have the so-called "gaps", i.e., missed parameters and characteristics. Another problem is that properties can describe any material with discrete values and by descriptive data such as text (e.g., the experience of use) and images (e.g., microstructure). These factors significantly complicate the creation of a source database that can be used for work with machine learning algorithms. In other words, the first step for using ML methods in the field of interest is estimating the possibility of collecting a dataset with clear, specific, and reliable data. The following steps include building a model and assessing its ability to adequately work with various machine learning algorithms to solve the problem [5]. In the case of modelling to predict material properties, the material characteristics (e.g., chemical composition) are called "input data".

In contrast, the properties (e.g., Yung's modulus, coercivity) are the "target" or "output data" [2]. Together, these data are called "vectors" or "fingerprints" in literature. During prognostic modelling, particular attention should be spent on the correct distribution of the collected dataset for training and test sampling and checking the correctness of the constructed model. For example, regression methods can be used if numerical values represent the target attribute (the property to be predicted). In contrast, classification methods are used for a categorical target (for example, a metal compound or not). In some cases, ensemble machine learning methods, which combine the results of individual methods, significantly increase the accuracy and adequacy of the model [1].

Finally, it is worth being noted that the possibility of using machine learning in materials science is limited and requires an assessment of the feasibility of its use in each case. Therefore, this work aims to estimate expediency using

ML methods to predict Sm-Co alloy's maximum energy product.

The main contribution of this paper can be summarized as follows:

- we have examined a boosting-based machine-learning model for solving Sm-Co alloy's maximum energy product prediction task;
- we have chosen the optimal parameters of the Gradient boosting regressor that is the basic of the developed model;
- we compare our results with existing ML-based methods and show the higher prediction accuracy of the proposed model.

The paper has the following structure. In section 2, we analysed existing works and showed the topicality of the stated task. In section 3, we describe the collected by us dataset used for modelling. In addition, we have described the proposed model and the number of performance indicators used for the evaluation of its efficiency. Modelling using Orange software as well as numerical and visual obtained results, are described in section 4. Summarization of the conducted research is in the Conclusion section.

2. State-of-the-arts

Sm-Co permanent magnets have the highest magnetic properties, second only to magnets based on the compound $\text{Nd}_2\text{Fe}_{14}\text{B}$ [22]. However, due to the high Curie temperature of the ferromagnetic phases SmCo_5 and $\text{Sm}_2\text{Co}_{17}$, they are indispensable when operating at high temperatures ($> 150^\circ\text{C}$). The magnetic properties of REM ferromagnetic materials almost reached the maximum possible values. A REM-based magnetic material's maximum possible energy product is determined by saturation magnetisation M_s : $(BH)_{\max} \leq (4\pi M_s)^2/2$ [23]. However, theoretical calculations and experimental results show that in the case of the formation of the nanostructured state, it is possible almost to double the magnetic properties of existing materials [24].

One possible way to form the nanostructured state in REM-based alloys is treatment under hydrogen using the HDDR process (hydrogenation, disproportionation, desorption, recombination) [25-27]. Over the last two decades, we have accumulated a large quantity of experimental data about phase transformations, crystallographic characteristics, texture parameters and microstructure evolution depending on the initial elemental composition of Sm-Co alloys and HDDR parameters (hydrogen pressure, maximum heating temperature, holding

time, cooling conditions, etc.) [28,29]. The final step of the study is to find the dependence of magnetic properties on the above parameters. Production of prototypes of sintered magnets and experimental establishment of their characteristics is a long and laborious process, with high financial and resource costs.

Literature data indicate the potential possibility of machine learning tools to forecast the magnetic properties of materials [30-33]. Considering the high cost of REM and the need for a significant number of experiments, we decided previously to evaluate the potential magnetic properties of our samples. As mentioned above, one of the most critical tasks in applying machine learning to solve material science problems is the availability of past data needed to create an original dataset and build a model and assess the real possibility of using this approach to solve a specific problem. Accordingly, in the first stage, we created a database based on literature sources in order to build an adequate model for predicting magnetic properties, which will be used in the future to predict the properties of our samples processed by the HDDR method.

During the creation of the database, we encountered several problems related to the completeness of the data in different sources, different approaches of the authors to the description of the microstructure parameters, etc., which are described in more detail in [12]. Based on the created database, we built a predictive model. We estimated the accuracy of various machine learning methods in predicting the coercive force of Sm-Co system ferromagnetic alloys [12]. It should be noted that the peculiarity of assessing the correctness of the prognostic model is that the data management model can "remember" each vector separately from the database. This case will demonstrate 100% accuracy of working with the same dataset but most likely will not work correctly with the other one. Therefore, reliable results are provided by k-fold cross-validation when randomly divided k-1 parts of the data set are used for training and one part for testing. Quantitative assessment of the accuracy of predictive models can be used using performance indicators of classification/regression methods, such as accuracy, sensitivity, specificity, Mean Absolute Error (MAE), Root Mean Squared Error (RMSE), coefficient of correlation (R), explained variance (R^2) etc. [1].

Our results showed that the best results in predicting the coercive force were obtained using a stacking ensemble model based on such heterogeneous elements as Neural Networks, AdaBoost, Gradient Boosting and Random Forest. The following values of Performance indicators Proposed ensemble model were obtained: $\text{MSE} = 44.223$; $\text{RMSE} = 6.650$; $\text{MAE} = 4.201$; and $R^2 = 0.636$ [12].

This work is a continuation of the research and involves the construction of a model for predicting the maximum energy product $(BH)_{\max}$ ferromagnetic alloys of the Sm-Co system. In this case, the main feature is the limited available source data. For comparison, of the more than 80 literature sources used to create the database, only about 25 contain measurement results $(BH)_{\max}$. In other words, a significant reduction in the vectors in the database takes place, as described below. It is known [34] that the amount of source data directly affects the accuracy of machine learning methods and is crucial in assessing the feasibility of such an approach. Based on this, we propose using the Boosting-Based Model to solve Sm-Co alloy's maximum energy product prediction task.

3. Materials and methods

We collected a database to predict the magnetic properties of REM permanent magnets using ML methods on the example of experimental study of Sm-Co ferromagnetic alloys available in the literature for the last decade. At that the methods of sample manufacturing do not take into account. Thus, the targets are magnetic properties, determined depending on chemical and phase composition, microstructure, texture and the average size of structural components. The following describes the features of dataset collection and the ML approach to solving the prediction task.

3.1. Dataset collection

The dataset for Sm-Co alloy's maximum energy product prediction task is a part of our database collected from literature data and described in detail in [12]. The input data (Fig. 1) included the content of chemical elements in the alloy, phase composition, material state, presence of texture and microstructure parameters. The main difference in this dataset from the full version of the database is the removal of vectors that don't contain the values of $(BH)_{\max}$ as the target.

In the result, we obtain the datasheet that contains only 190 vectors compared to 420 in the full version. Thirty input attributes describe each included observation. The elements (the content of Sm, Co, Fe, Cu, Zr and total amount such REM metals as La, Ce and Pr), the average size of structural components and maximum energy product are presented as numerical, while the rest of the data in a categorical way. The data on phase composition contains information about the main ferromagnetic and second phases (SmCo_5 , $\text{Sm}_2\text{Co}_{17}$, Sm_2Co_7 , SmCo_7 , SmCo_3 , Sm_2O_3 , Co, Fe, FeCo,

and Zr-rich phases). Powder, sintered magnet or ribbon represents the state of the material. The microstructure parameters included type (lamellar, flake, nanocrystalline, and cellular), average size, homogeneity and regularity. In addition, each vector contains information about the presence of texture.

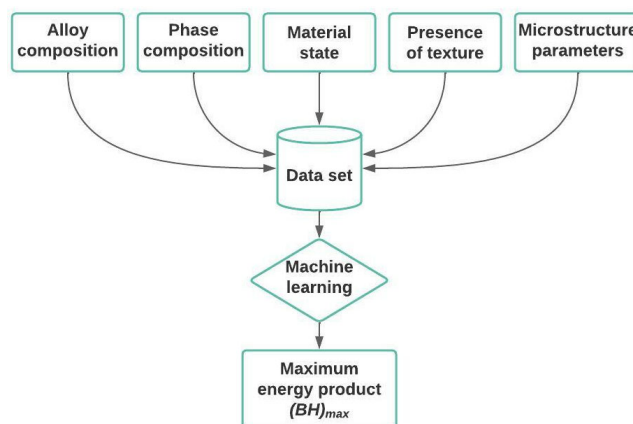


Fig. 1. Schematic representation of the collected dataset

3.2. Boosting model

The modern development of artificial intelligence tools and its application to solve applied materials science problems provides a reduction in time, cost reduction, material costs, and so on. However, the features of each specific situation determine the search for the most optimal method of its solution based on the accuracy of work, the speed of learning time of the model, minimizing the computing resources required for the operation of a method [34]. In the case of limited amounts of data, which is very typical for various materials science problems in the first place is the accuracy of the problem solving [35].

Many developments and studies on machine learning methods to solve regression or classification problems demonstrate the low accuracy of single-based methods [36]. One possible solution to avoid this problem is to apply a strategy of assembling machine learning methods. There are three most commonly used options: bagging, boosting and stacking.

In this paper, the authors investigate the boosting strategy of integrating machine learning methods to improve the forecast accuracy of the Sm-Co alloy's maximum energy product [37]. It involves constructing and using a set of weak classifiers that classify objects better than random guessing and taking their response into account when constructing stronger classifiers. Thus, the boosting hypothesis involves

an iterative process of learning weak classifiers and collecting them into one robust classifier.

This approach aims to reduce the supervised machine learning algorithm variance significantly. As a result, it substantially increases the accuracy of the work of classifiers or regressors based on this ensemble strategy.

Among the disadvantages of this approach should be noted the iterative nature of the learning procedure and the consistent operation of the boosting algorithm, which significantly affects the speed of such methods. However, in cases where the priority is the accuracy of the work and data sets for processing – small, such a strategy is entirely justified.

Among the many such methods, which essentially differ only in some algorithm elements, the authors used and studied one of the earliest busting methods of machine learning – Gradient Boosting.

The Gradient Boosting method is based on the idea of consistent use of weak models and taking into account the outputs of the previous one to increase the accuracy of the next one. Such an approach should provide an opportunity to learn each subsequent model from the mistakes of the previous one.

Decision trees are usually used as weak classifiers.

An essential step of the algorithm is to determine the stage of its stop. That is, at what phase of consistent inclusion and training of weak classifiers to build the strongest, i.e., the most accurate, should be stopped. In this case, when determining and minimizing the loss function, a gradient descent algorithm is used, which is fast and relatively accurate and provides a quick search for the minimum value of the user-selected loss function.

3.3. Performance indicators

Estimation of the accuracy of the studied model in solving the problem of forecasting Sm-Co alloy's maximum energy product was performed using several indicators, in particular [38]:

1. MSE (Mean Square Error)

$$MSE = \frac{1}{N} \sum_{i=1}^N (y_i^{pred} - y_i^{true})^2 \tag{1}$$

2. RMSE (Root Mean Square Error)

$$RMSE = \sqrt{\frac{\sum_{i=1}^N (y_i^{pred} - y_i^{true})^2}{N}} \tag{2}$$

3. MAE (Mean Absolute Error)

$$MAE = \frac{1}{T} \sum_{i=1}^N |y_i^{pred} - y_i^{true}| \tag{3}$$

4. R2 (Coefficient of determination)

$$R2 = 1 - \frac{\sigma^2}{\sigma_y^2} \tag{4}$$

where: y_i^{true} are the true values of the Sm-Co alloy's maximum energy product; y_i^{pred} are the respected predicted values of the Sm-Co alloy's maximum energy product; $i = 1, N$ is the current point; N is the number of observed vectors; σ_y^2 is the total sum of squares and σ^2 is the sum of squares of residuals.

4. Results and discussion

4.1. Modelling

The simulation of the work of the boosting ensemble took place using the environment of intellectual analysis and data visualization – Orange. This approach is explained by: the ease of use of this program without the need for deep knowledge of the user in the field of machine learning; construction of schemes of data analysis and visualization using visual programming, which provides the possibility of using the program by specialists without programming experience; availability of additional procedures for data processing, feature selection, cross-validation, etc., which

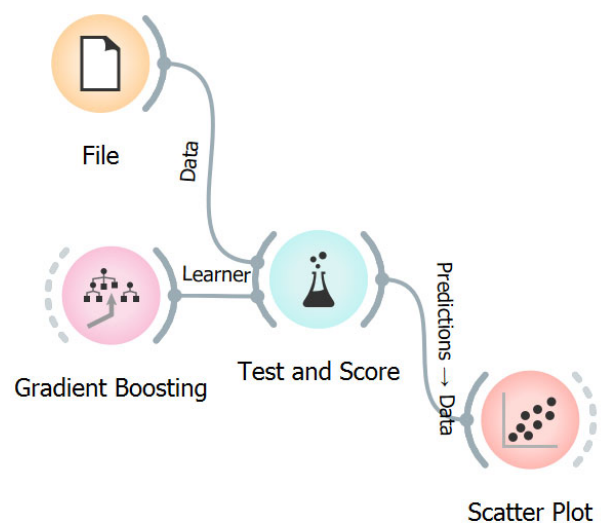


Fig. 2. Flowchart of the modelling process in Orange

significantly simplifies the work on data analysis; a wide variety of means and tools for visualization of the obtained results for their optimal presentation; possibility to select the necessary parameters of the model in the dialogue mode; high speed of work due to the optimized operation of implemented machine learning methods, etc. The scheme of the modelling process is shown in Figure 2.

The studied models' effectiveness was evaluated using the ten-fold cross-validation procedure to ensure the reliability of the simulation results (Fig. 3).

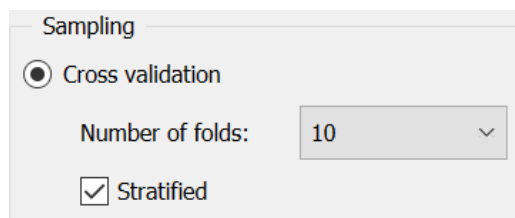


Fig. 3. 10-fold cross validation

For a comprehensive analysis of the results obtained, the performance evaluation of the investigated models was performed using four different accuracy indicators (1)-(4).

The results of different machine learning models have been visualized in the form of scatter plots for the possibility of comparing the effectiveness of their work.

4.2. Results

As a result of modelling using 10-fold cross-validation, the values of indicators (1)-(4) were obtained, summarized in Table 1.

Table 1.

Modelling results				
Method	MSE	RMSE	MAE	R2
Gradient Boosting	17.966	4.239	2.885	0.798

It should be noted that the values of the optimal parameters of the method are as follows:

- maximal number of trees = 10000;
- limit depth of individual trees = 5;
- minimal number of trees for splitting subsets = 2;
- learning rate = 0.1.

4.3. Comparison and discussion

Comparison of different machine learning algorithms based on (1)-(4) indicators is given in Table 2.

Table 2.

Comparison of different machine learning algorithms

Method	MSE	RMSE	MAE	R2
Tree	41.232	6.421	4.692	0.556
SVM	39.048	6.249	5.128	0.580
SGD	33.230	5.765	4.162	0.642
Linear regression	32.500	5.701	4.356	0.650
AdaBoost	20.362	4.512	2.981	0.781
Random Forest	20.049	4.478	3.162	0.784
Gradient Boosting	17.966	4.239	2.885	0.798

From the results presented in Table 2, we can say the following:

1. all studied models demonstrate adequacy (coefficient of determination greater than 0.5). The obtained result suggests the possibility of using machine learning tools to solve the problem of the Sm-Co alloy's maximum energy product prediction;
2. the most accurate results are obtained when using ensemble methods. This confirms the hypothesis that the strategy of the ensemble in solving the problem has been fully justified;
3. the highest accuracy indicators for all four metrics (1)-(4) during the solution of the problem was obtained based on the use of a boosting model based on Gradient Boosting.

The Scatter Plot widget of the Orange software was used to illustrate the results of the research methods. It should be noted that Figure 4 shows graphs for only three ensemble methods, as they provide the highest forecast accuracy of the Sm-Co alloy's maximum energy product.

Scatter Plot shows the ratio of two variables in the form of points on the Cartesian space. In this case, the original values of the required property along to OX axis and the predicted values obtained by the studied algorithm of machine learning along the OY axis are demonstrated. The correlation field formed by such a graph can illustrate the accuracy level of the selected machine learning model. The narrower the correlation field (from the side diagonal), the more accurate the chosen machine learning algorithm. Accordingly, the wide correlation field shows the regressor's poor properties in predicting the desired result.

As shown in Figure 4a, the studied boosting model demonstrates the smallest scatter of values – the highest correlation field of the other two ensemble methods.

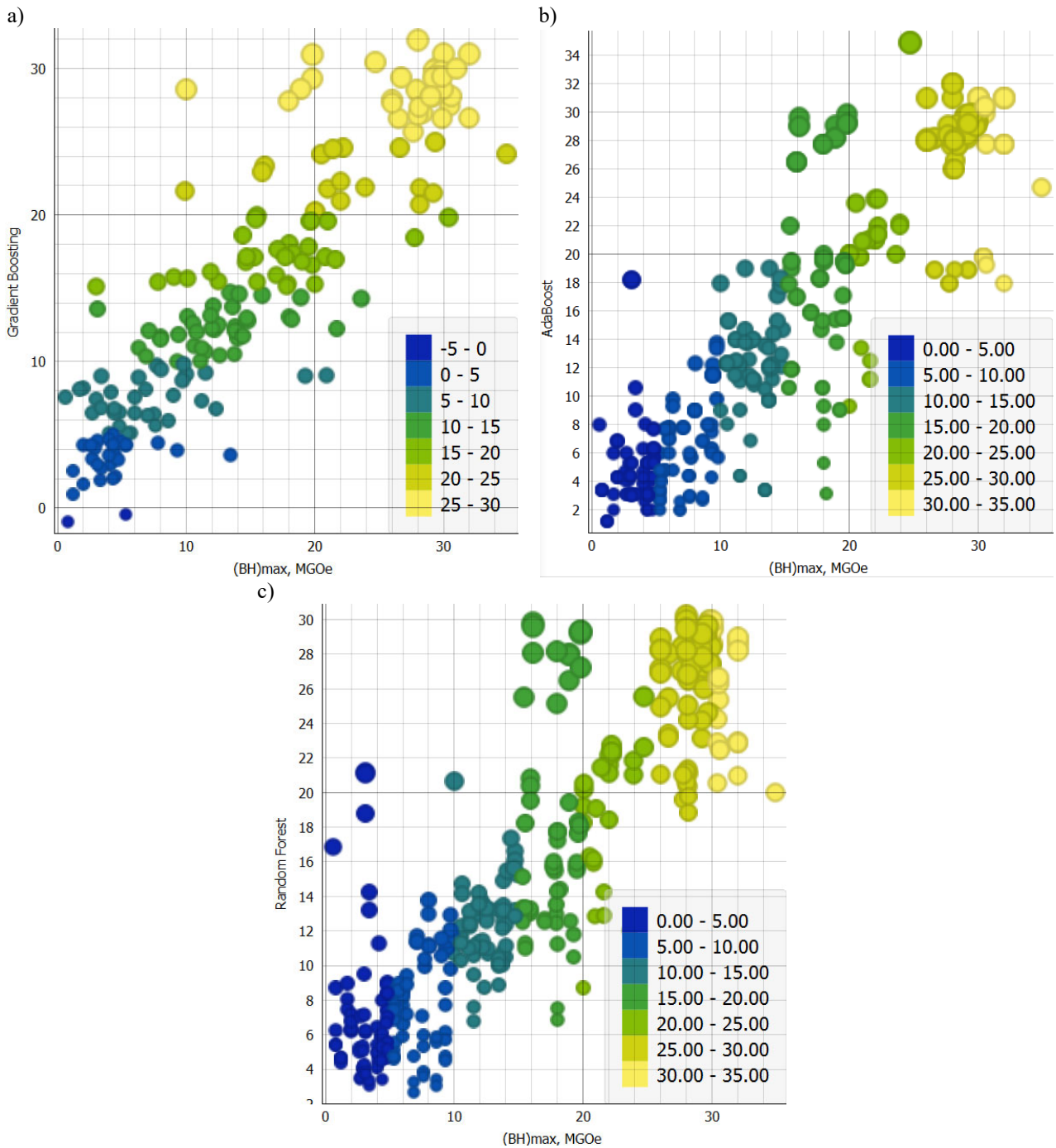


Fig. 4. Flowchart of the modelling process in Orange

This result is confirmed by the numerical estimates of accuracy based on (1)-(4) obtained in Table 2. Therefore, the ensemble model based on boosting can be used when solving applications for forecasting Sm-Co alloy's maximum energy product.

5. Conclusions

This paper considers the problem of the Sm-Co alloy's maximum energy product prediction. The authors propose an approach based on ensemble learning to solve it. Because

classical machine learning methods do not always provide a sufficient level of accuracy when solving the regression problem (as confirmed in the paper), the authors used a boosting strategy for assembling machine learning methods, namely the Gradient Boosting method. Building a boosting model based on several weak sub-models, each of which considers the results of previous work, significantly increases the accuracy of solving the problem. This is confirmed using an actual data set collected by the authors.

According to the obtained results, all studied models demonstrate adequacy (coefficient of determination greater than 0.5). The obtained result suggests the possibility of using machine learning tools to solve the problem of the Sm-Co alloy's maximum energy product prediction. The most accurate results of solving Sm-Co alloy's maximum energy product prediction task were obtained using boosting machine learning model. The highest accuracy indicators for all four metrics (1)-(4) during the solving of the stated task was obtained based on the use of a boosting model based on Gradient Boosting. In addition; we show the results of the investigated methods in graphical form. It is shown the same results as in numerical form.

Given that the studied boosting model of machine learning provides high prediction accuracy, this reveals several advantages of their use in solving applied problems of computational material science. Furthermore, using the Orange modelling environment provides a simple and intuitive interface for using the studied methods. The proposed prediction approach significantly reduces the time and resource costs associated with studying expensive ferromagnetic materials based on rare earth metals.

Among the limitations of the proposed approach, it should be emphasised that the boosting strategy of machine learning compared to single-based machine learning algorithms, requires significantly more computing and time resources to implement the model learning procedure.

Further research will be conducted to apply other strategies to improve the accuracy of the problem of the Sm-Co alloy's maximum energy product prediction, particularly the use of artificial neural network stacking.

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