Machine Learning Approaches to Predicting and Understanding the Mechanical Properties of Steels

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Abstract

The mechanical properties are essential for structural materials. A dataset consists of 102 carbon steel and 258 low-alloy steel was built from the NIMS steel fatigue dataset. And five machine learning algorithms were applied on the dataset to predict the mechanical properties, including fatigue strength, tensile strength, fracture strength, and hardness of steels. Random forest shows a tremendous predictive power of those properties of steels. The prominent features of those properties were selected based on random forest, and symbolic regressions, the tempering temperature and the alloying elements of carbon, chromium, and molybdenum were shown to play essential roles on the mechanical properties. Besides, the mathematic expressions were generated via symbolic regression, and the expression can directly predict the mechanical properties with heat treatment conditions and compositions. The symbolic regression algorithm shows excellent potential in feature selection and expression discovery in materials science.

1. Introduction

Seeking structure-property relationships is an alternative and accepted approach to new materials discovery. However, the comprehensive mechanisms are still unclear due to the diversity and complexity of materials. Discovering new materials through experiments and computations in the ‘trial-and-error’ method is a slow and formidable task. A large amount of data has been generated by the experiments and computations in materials discovery. Materials science becomes a data-driven science with the advance of big data and artificial intelligence (AI) in the last few years, it utilizes technologies such as data mining and machine learning for materials research.

Machine learning and materials big-data provide the foundations for a data-driven materials paradigm; it takes advantage of data mining tools and applies them to experimental and computational approaches for materials discovery. In recent years, material informatics have been developed rapidly. The necessity of materials informatics was emphasized by the Materials Genome Initiative (MGI) project in 2011. The American government wanted to develop an infrastructure to accelerate the discovery, development, and deployment of advanced materials with the materials informatics approach [1]. Materials data can be used to seek quantitative structure-property relationships and build models for new materials synthesis. For example, Homer et al. [2] and Zhu et al. [3] employed ML tools to investigate ground boundaries in crystalline materials. Raccuglia et al. [4] demonstrated a ML strategy to elucidate the features influencing reaction and predict successful reactions with historical experiments (including successful and failure). Agrawal et al. [5] used ML algorithms to predict the fatigue strength of steel with the NIMS materials database. The machine learning applications make a substantial impact and guide the experimental discovery in industry. However, machine learning algorithms Agrawal used are black boxes. A mathematic expression is required for material design and properties prediction of steels.

The purpose of this work is to predict the mechanical properties of steel via a machine learning technique. Five machine learning algorithms were employed and compared to build a predictive model with high accuracy. A white-box algorithm, symbolic regression was also employed to seek the compositions-
structure-property relationships of steels. Also, by using symbolic regression, three prominent features have been selected, and they showed durable predictive power.

2. Data resource

Publicly available fatigue dataset for steels collected by Japan National Institute of Material Science (NIMS) [6] was used in this work. It is one of the most massive datasets in the world with compositions and product features. It also has data on the mechanical properties of steels at room temperature, including fatigue strength, tensile strength, fracture strength, and hardness. Fatigue strength is the highest stress that a material can withstand for a given number of cycles without breaking and is an extremely critical property of steels for industrial application. The rotating bending fatigue strength at $10^7$ cycles was used as fatigue strength for prediction in this work.

The fatigue testing conditions, including frequency, loading condition, and specimen dimensions, might significantly affect fatigue behavior. Thus, only 393 samples under the same testing condition shown as [7] were studied in this work. The chosen samples from NIMS consisted of 113 carbon steel, 258 low-alloy steel, and 22 stainless steel. Those steels were described with chemical compositions, processing parameters, inclusion parameters, and mechanical properties. The compositions include nine alloying elements (C, Si, Mn, P, S, Ni, Cr, Cu, Mo) and Fe. The processing parameters consist of reduction ratio (ingot to the bar), heat treatment parameters (temperature and holing time) in normalizing, quenching, and tempering. The inclusion parameters are the area fraction of non-metallic inclusions, including dA (inclusions deformed by plastic work), dB (inclusions occurring in discontinuous arrays), and dC (isolated inclusions). In particular, the features related to heat treatment were processed as follows:

(1) The holding time in normalizing, quenching, and tempering are constant values of 30 min, 30 min, and 60 min in the raw data, respectively. These three features thus were excluded.

(2) The steels not normalized (SC25 steels) or not quenched and tempered (stainless steels) were excluded.

The processed training set has 360 samples, 16 variables consist of nine alloying elements, one reduction ratio, three heat treatment temperatures, three inclusions and four target properties (fatigue strength, tensile strength, fracture strength, and hardness). The minimum and maximum values of each feature are shown in Table 1. The learned ML models were examined by ten cross-validation method.

Table 1. Training dataset features for NIMS fatigue data

| Features            | Description            | Min    | Max    | Mean   | StdDev |
|---------------------|------------------------|--------|--------|--------|--------|
| NT                  | Normalizing Temperature| 825    | 900    | 865.6  | 17.37  |
| QT                  | Quenching Temperature  | 825    | 865    | 848.2  | 9.86   |
| TT                  | Tempering Temperature  | 550    | 680    | 605    | 42.4   |
| C ($x_1$)           | wt% of Carbon          | 0.28   | 0.57   | 0.407  | 0.061  |
| Si ($x_2$)          | wt% of Silicon         | 0.16   | 0.35   | 0.258  | 0.034  |
| Mn ($x_3$)          | wt% of Manganese       | 0.37   | 1.3    | 0.849  | 0.294  |
| P ($x_4$)           | wt% of Phosphorus      | 0.007  | 0.031  | 0.016  | 0.005  |
| S ($x_5$)           | wt% of Sulphur         | 0.003  | 0.03   | 0.014  | 0.006  |
| Ni ($x_6$)          | wt% of Nickel          | 0.01   | 2.78   | 0.548  | 0.899  |
| Cr ($x_7$)          | wt% of Chromium        | 0.01   | 1.12   | 0.556  | 0.419  |
| Cu ($x_8$)          | wt% of Copper          | 0.01   | 0.22   | 0.064  | 0.045  |
| Mo ($x_9$)          | wt% of Molybdenum      | 0      | 0.24   | 0.066  | 0.089  |
| Fe ($100 - \sum_{i=1}^9 x_i$) | wt% of Iron          | Balanced |
| RR                  | Reduction ration       | 420    | 5530   | 971.2  | 601.4  |
| dA                  | Plastic work-inclusions| 0      | 0.13   | 0.047  | 0.032  |
| dB                  | discontinuous array-inclusions | 0 | 0.05 | 0.003 | 0.009 |
| dC                  | isolated inclusions   | 0      | 0.04   | 0.008  | 0.01   |
3. Methods

High dimensional feature space will lead to lousy robustness and generalization ability of ML algorithms, some ML algorithms thus have been developed to select relevant features based on their importance when building the models. In this work, random forest and symbolic regression, which can select features, were employed.

3.1 Random Forest

Random Forest is a useful tool widely used in practice. It is an ensemble ML algorithm shown as Algorithms 1 which works as follows: a bootstrap sample (in-bag observations) from the training set was randomly selected with replacement to build a decision tree, out-of-bag (OOB) observations which were not used for build decision tree can be utilized to estimate the prediction performance of the corresponding tree, then a powerful RF model was formed by averaging the predictions of all individual learned trees [8].

Algorithm 1: Random Forest Regression

Input: Training set $T$, features $F$, number of trees in forest $n$ (here $n = 100$).
Output: A random forest

1. function RandomForest ($T$, $F$) for $k=1$ to $n$ trees
2. let $S_i$ be a bootstrap sample of $S$ with replacement
3. apply RandomForest on $S_i$ to obtain a model $M_k$
4. end for
5. return a RandomForest model $M$ composed of $n$ trees $M_k$
6. end function

A random-selected subset $f$ of features $F$ were examined at each node of every decision tree. The node splits on the best feature in the subset $f$ according to the impurity decrease criterion. Impurity decrease is measuring how effective each feature is at reducing the variance between predicting and actual values when creating a regression decision tree. The impurity decrease from each feature can be averaged to get a mean impurity decrease value in the final forest. The random forest thus can be used to compute the importance of features (RFI) based on mean impurity decrease, the more a feature decreases the impurity, the more prominent the feature is.

3.2 Symbolic Regression

Besides, an explainable algorithm, symbolic regression, was introduced in this work. Symbolic regression is a machine learning algorithm that aims to identify a mathematical expression that accurately describes an input-output relationship. There exists a massive number of potential expressions with all available features. Thus, a globally optimal solution given by exhaustive search is not available [9]. The SR utilizes genetic programming (GP) to search for a local optimal expression from the model space efficiently. Each generation of GP explores a set of solutions, commonly called a population. SR begins with building a population of random solutions. The performance of all solutions is assessed based on the relative root mean square error (RMSE). A new-generation population is then generated by crossover and mutation operators. Each solution in SR is described
as an expression tree, crossover (here 80% probability) is an operator of recombining two parents by using subtrees to generate a new child solution, mutation (20% probability) introduces random features or functions into parent’s expression tree. The SR model was obtained as the solution with the lowest RRMSE among all generations (10000).

**Algorithm 2: Symbolic Regression**

**Input:** Training set $T$, features $F$, mathematic operator $M$, probability of crossover (80%) and mutation (20%), population size (1000), the number of generations (10000)

**Output:** A mathematic expression

1. randomly choose an initial population of solutions fitted by $F$ and $M$
2. evaluate the root mean square error of each solution

Repeat

3. select the solution with the lowest root mean square error
4. generate a new-generation population by the crossover and mutation
5. evaluate the root mean square error of each solution in the new generation

until the stopping criterion (10000 generations)

7. return a mathematic expression with the lowest RMSE among 10000 generations

8. end

GP is a stochastic optimization method, and its results largely depend on its random initial population. One hundred independent GP runs are conducted for the SR problem in this work to obtain a better expression. In GP runs, solutions integrating redundant features will perform worse than solutions using only relevant features; those redundant features will have lower chances of being chosen to produce children. The features presence thus can indicate the importance of features; this presence-importance (PI) of a feature ($f_i$) is computed as a fraction of the solutions containing this feature. Enhanced importance, termed as symbolic regression importance (SRI), was proposed based on 100 independent runs in this work. SRI was estimated via weighting the PI of features with the correlation coefficient of each SR result ($M_i$).

$$SRI(f_i) = \sum_{i=1}^{100} [PI(f_i, M_i) R^2(M_i)]$$  

(1)

3.3 Validation and Evaluation

Ten-folds cross-validation was used in this work to evaluate the performance of learned models on the unseen data. The pre-processed samples were randomly divided into ten parts, 90% training samples, and 10% testing samples. Repeating this process ten times, and all samples were tested.

The predictive power of a ML model on the testing samples can be explained by the correlation coefficient (R), and relative root mean square errors (RRMSE). These criteria can capture the difference between predicted and actual fatigue strength

$$R = \frac{\sum_{i=1}^{n} (y_i-\bar{y})(\hat{y}_i-\bar{\hat{y}})}{\sqrt{\sum_{i=1}^{n} (y_i-\bar{y})^2 \sum_{i=1}^{n} (\hat{y}_i-\bar{\hat{y}})^2}}$$  

(2)

$$RRMSE = \frac{1}{n} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 \bar{y}_i$$  

(3)

where $n$ is the number of training or testing samples, $y$, $\hat{y}$ and $\bar{y}$ denotes the actual value, predicted value, and average value, respectively. The performance of cross-validation can be computed as the average value of ten tests. $R$ is between 0 and 1, and a value of 1 indicates a perfect prediction. RRMSE is non-negative, and a value of 0 indicates a perfect fit. In general, a model with higher $R$ and lower RRMSE is better [10].
4. Results and discussion

4.1 ML Model with All Features

RF and other four popular ML algorithms including linear least square (LLS), k-nearest neighbors (KNN), architecture-neutral network (ANN) and support vector machine (SVM) were applied to the training set without feature selection. The R and RRMSE value of each model were computed and compared in Figure 1, the predicted values of the best model for each property were plotted against the measured property as well.

The RF shows greater predictive power than other algorithms on the fatigue strength ($R = 0.9635$, $RRMSE = 27.26\%$) and fracture strength ($R = 0.9716$, $RRMSE = 23.85\%$). While the best model for the tensile strength ($R = 0.9831$, $RRMSE = 19.86\%$) and hardness ($R = 0.9817$, $RRMSE = 20.11\%$) is the ANN algorithm.

4.2 Feature Selection

The RFI and SRI values of each feature were compared on the entire dataset, the feature importance for the four mechanical properties were shown in Figures 2 (a)-(d). Based on the RFI values, the alloying elements of molybdenum and chromium are the most important features followed by the tempering and normalizing temperatures, and these four features show much higher importance than the rest. The SRI values showed that the tempering temperatures have the highest effect, and the alloying elements of molybdenum, chromium, and carbon has a greater influence than other alloying elements. Two subsets of feature thus were determined by the RFI (TT, NT, Cr, Mo) and SRI (TT, C, Cr, Mo) values.

Five ML algorithms were applied to examine the predictive power of those two subsets for four properties. The cross-validation R-value of models for each property was compared, and the predicted values of the best model against the measured value for each property were plotted in Figure 3. The RF algorithm outperforms other algorithms on these two subsets, and RF models on SRI subset performs the best among ten models for each property. Models on the SRI subset have a slightly smaller R-value than the model without feature selection for all target properties, SRI-subset is therefore an appropriate subset to be used in the ML procedure. The RF model on SRI-subset can predict the four target properties well with relatively high predictive accuracy ($R > 0.9550$, $RRMSE < 28.00\%$).
Figure. 1 (a) The comparison of RF, LLS, KNN, ANN and SVM for fatigue strength without feature selection, and the performance of the best model RF@All; (b) The comparison of RF, LLS, KNN, ANN and SVM for tensile strength without feature selection, and the performance of the best model ANN@All; (c) The comparison of RF, LLS, KNN, ANN and SVM for fracture strength without feature selection, and the performance of the best model RF@All; (d) The comparison of RF, LLS, KNN, ANN and SVM for hardness without feature selection, and the performance of the best model ANN@All.

Figure. 2 The normalized (a) random forest importance (RFI) and (b) symbolic regression importance (SRI) of each NIMS feature for fatigue strength, tensile strength, fracture strength, and hardness.
Figure. 3 (a) The comparison of RF, LLS, KNN, ANN and SVM for fatigue strength on RFI and SRI subset, and the performance of the best model RF@SRI; (b) The comparison of RF, LLS, KNN, ANN and SVM for tensile strength on RFI and SRI subset, and the performance of the best model RF@SRI; (c) The comparison of RF, LLS, KNN, ANN and SVM for fracture strength on RFI and SRI subset, and the performance of the best model RF@SRI; (d) The comparison of RF, LLS, KNN, ANN and SVM for hardness on RFI and SRI subset, and the performance of the best model RF@SRI.

Figure. 4 The predicted values of SR expressions against the measured values for (a) fatigue strength, (b) tensile strength, (c) fracture strength and (d) hardness.
4.3 Mathematical Expressions and Applications

Mathematical expressions are required to directly predict the mechanical properties with the heat treatment conditions and compositions in the industry. SR runs on the entire dataset gave the mathematical expressions for fatigue strength, tensile strength, fracture strength, and hardness as equations (4)-(7), respectively.

\[
\text{Fatigue} = -0.4737TT - 0.9951TT \cdot C + 1283\sqrt{C} + 51.80\sqrt{Mn} + 27.10Ni + 70.05Cr + 49.42\sqrt{Cr} + 74.41\sqrt{Mo} + 61.4
\]  
(4)

\[
\text{Tensile} = -1.418TT - 1.049TT \cdot C + 1846\sqrt{C} + 76.06Mn - 32.91Ni + 131.2\sqrt{Ni} + 219.6Cr + 145.4\sqrt{Mo} + 592.1
\]  
(5)

\[
\text{Fracture} = -2.863TT \cdot C + 2678\sqrt{C} + 236.3C \cdot Cr + 80.45Mn + 92.19Ni - 74.86\sqrt{Ni} + 170.6\sqrt{Cr} - 521.0Mo + 402.9\sqrt{Mo} + 371.6
\]  
(6)

\[
\text{Hardness} = -0.5853TT + 263.5\sqrt{C} + 49.95C \cdot Mn - 13.57Ni + 40.45\sqrt{Ni} + 29.49Cr + 45.76\sqrt{Cr} - 122.7Mo + 104.4\sqrt{Mo} + 391.8
\]  
(7)

Those equations show strong predictive power (R > 0.9500, RRMSE < 31.00%) in the Figure 4. Based on the above equations, the tempering temperature was shown to negatively correlated with the mechanical properties of those steels, and lower tempering temperatures were suggested to improve the strength of steels. The normalizing and quenching temperature was positively correlated with the mechanical properties, and the strength will increase with the increasing of normalizing and quenching temperature. Also, the alloying elements carbon, which exists as the interstitial solution in steels, can improve the mechanical properties of steels. The alloying elements of chromium, nickel, manganese, and molybdenum, which exist as substitutional solid solutions, also can strengthen the steels.

4.4 A case of designing high-strength steels

With given ML models and mathematical expression, new steels can be developed with high strength and hardness. In carbon and low-alloy steels, the lowest tempering temperature is 550 °C for forming tempering sorbate. The maximum content of C, Cr, Ni, Mn, and Mo in the training set is 0.57%, 1.12%, 2.78%, and 0.24%, respectively. Thus, new steel (NSA) with high strength and hardness might be produced with the conditions shown in Table 2 based on equations (4)-(7). The computing fatigue strength (759.1 MPa), tensile strength (1421.1 MPa), fracture strength (2135.7 MPa), and hardness (438.7 HV) of NSA are much higher than then corresponding maximum value in the dataset.

| TT     | C    | Cr   | Ni    | Mn    | Mo    | Other features |
|--------|------|------|-------|-------|-------|----------------|
| 550 °C | 0.57 | 1.12 | 2.78  | 1.3   | 0.24  | Mean value     |

| Properties       | The maximum value in the dataset | The estimated value of NSA |
|------------------|----------------------------------|-----------------------------|
| Fatigue Strength (MPa) | 643                               | 759.1                       |
| Tensile Strength (MPa)    | 1206                              | 1421.1                      |
| Fracture Strength (MPa)    | 1931                              | 2135.7                      |
| Hardness (HV)              | 380                               | 438.7                       |
4.5 ML model based on atomic property

Above ML models cannot predict the mechanical properties of steels that contain alloying elements (such as V and W) not mentioned in the dataset. Atomic properties can be introduced to construct ML models to improve the generalization ability. Iron is the matrix of iron-alloys, alloying elements exist as solid solutions, and metal carbides are the primary precipitates in the matrix. Thus, the atomic percentage of Iron (a_{Fe}), tempering temperatures (the prominent feature besides compositions) and the atomic properties shown in Table 4 were studied in the current work.

Table 4 Atomic properties used in this work

| Features          | Description                               | Formula                                      |
|-------------------|-------------------------------------------|----------------------------------------------|
| $t_r$             | Total atomic radius                       | $\sum_{i=1}^{n} a_i r_i$                     |
| d_{r,Fe}          | Atomic radius difference (Iron-based)     | $\sqrt{\sum_{i=1}^{n} a_i (1 - \frac{r_i}{r_{Fe}})^2}$ |
| tVEC              | Total Valance Electron                    | $\sum_{i=1}^{n} a_i VEC_i$                   |
| d_{VEC,Fe}        | Valance Electron difference (Iron-based)  | $\sqrt{\sum_{i=1}^{n} a_i (1 - \frac{VEC_i}{VEC_{Fe}})^2}$ |
| d_{VEC,C}         | Valance Electron difference (Carbon-based)| $\sqrt{\sum_{i=1}^{n} a_i (1 - \frac{VEC_i}{VEC_{C}})^2}$ |
| $t_\chi$          | Total Pauling Electronegativity           | $\sum_{i=1}^{n} a_i \chi_i$                 |
| d_{r,Fe}          | Electronegativity difference (Iron-based) | $\sqrt{\sum_{i=1}^{n} a_i (1 - \frac{\chi_i}{\chi_{Fe}})^2}$ |
| d_{r,C}           | Electronegativity difference (Carbon-based)| $\sqrt{\sum_{i=1}^{n} a_i (1 - \frac{\chi_i}{\chi_{C}})^2}$ |

RFI and SRI method was applied to those features, and RF models were built with these two subsets. The RFI subset consisted of $t_{VEC}$, $d_{VEC,Fe}$, $d_{VEC,C}$, and TT for fatigue strength and hardness, while $a_{Fe}$ appeared instead of $d_{VEC,Fe}$ for tensile strength and fracture stress. The SRI values showed that $d_{VEC,C}$, $d_{r,Fe}$, $a_{Fe}$, and TT have the highest effect on the four mechanical properties, and the SRI subset has more durable predictive power than RFI model. SR runs gave four expressions of mechanical properties as equations (8)-(11) with those atomic features.

Fatigue = $-0.878TT - 986.4\sqrt{a_{Fe}} + 381.5t_r + 13314d_{r,Fe} - 29187d_{r,C} + 8525t_{VEC} + 38528d_{VEC,C} - 77556$  
(8)

Tensile = $-1.823TT - 9364a_{Fe} + 769.6t_r + 29864d_{r,Fe} - 37367d_{r,C} + 16199t_{VEC} + 74228d_{VEC,C} - 169513$  
(9)

Fracture = $-1.145TT - 9727\sqrt{a_{Fe}} - 21742d_{r,Fe} + 34832d_{r,C} - 12539d_{r,C} + 3658d_{VEC,Fe} + 53303d_{VEC,C} - 11881$  
(10)

Hardness = $-0.57TT - 1227a_{Fe} - 2048d_{r,Fe} + 6943d_{r,C} + 1093d_{VEC,Fe} + 16325d_{VEC,C} - 6697$  
(11)
Figure 5 The predicted values of RF model on SRI subset and SR expressions based on atomic properties against the measured values for (a) fatigue strength, (b) tensile strength, (c) fracture strength and (d) hardness.

5. Conclusion

In this work, we compared serval ML models for predicting mechanical properties of steels and construed a new method based on the symbolic regression to choose the most important features for mechanical properties. The proposed method shows that tempering temperature, weight-percentage of carbon, chromium, and molybdenum play important roles in the mechanical properties of steels. A random forest built with those features can get a high validation accuracy ($R > 0.9550$, RRMSE < 28.00%).

Four mathematic expressions were generated via SR, and the expressions suggest that low tempering temperature, will benefit the fatigue strength. The alloying elements carbon, which exists as the interstitial solution in steels, can improve the mechanical properties of steels. The alloying elements of chromium, nickel, manganese, and molybdenum, which exist as substitutional solid solutions, also can strengthen the steels. Based on the SR expressions, one can directly predict the mechanical properties with heat treatment conditions and compositions. Also, mathematical expression and RF models based on atomic properties were also built for general purpose. The symbolic regression algorithm shows excellent potential in feature selection and expression discovery.
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Reference

[1] Green M. L., et al. Fulfilling the promise of the materials genome initiative with high-throughput experimental methodologies. Applied Physics Reviews 4.1 (2017): 011105.

[2] Homer E. R., et al. Machine-learning informed representations for grain boundary structures. Frontiers in Materials 6 (2019): 168.

[3] Zhu Q., et al. Predicting phase behavior of grain boundaries with evolutionary search and machine learning. Nature communications 9.1 (2018): 1-9.

[4] Raccuglia P., et al. Machine-learning-assisted materials discovery using failed experiments. Nature 533.7601 (2016): 73-76.

[5] Agrawal A., et al. Exploration of data science techniques to predict fatigue strength of steel from composition and processing parameters. Integrating Materials and Manufacturing Innovation 3.1 (2014): 8.

[6] NIMS Fatigue Data Sheet: these data sheets are available at (http://mits.nims.go.jp/)

[7] NIMS Fatigue Data Sheet No.1, 1978

[8] Liaw A., and Matthew W.. Classification and regression by randomForest. R news 2.3 (2002): 18-22.

[9] Billard L., and Edwin D.. Symbolic regression analysis. Classification, Clustering, and Data Analysis. Springer, Berlin, Heidelberg, 2002. 281-288.

[10] Alpaydin E.. Introduction to machine learning. MIT press, 2014.