# The prediction of structural properties of Ni-Ti shape memory alloy by the supervised machine learning methods

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#### Abstract

Shape memory alloys (SMAs) possess unique properties, namely, they retain their original form after loading while being, for instance, heated. The structural properties of pseudoelastic NiTi SMA, such as the dependencies of stress and strain range upon the number of loading cycles, were studied by employing the methods of supervised machine learning (ML). The obtained results are quite accurate, which can be seen from the calculated mean average error (MSE) and root mean squared error (RMSE). In general, ML methods can be utilized to solve such kinds of tasks very efficiently.

#### **Keywords**

machine learning, neural network, random forest, NiTi shape memory alloy, stress and strain ranges

## 1. Introduction

Shape memory alloys (SMAs) 'memorise' or retain their initial shape when under the action of thermomechanical or magnetic fields [1]. SMAs have gained vast attention recently in a wide range of applications, that are based on their peculiar properties, namely, in products [2], structural elements [3], automotive [4], aerospace [5, 6], mini actuators and micro-electromechanical systems (MEMS) [7, 8], etc. Therefore, due to their ubiquitous widespread, it is highly important to study their structural properties, namely, the dependencies of stress and strain upon the number of loading cycles. A number of related computer modelling and simulations was performed in the studies [9-11]. Since the testing procedures are often quite costly and time-consuming, it is advisable to use the methods of artificial intelligence (AI), specifically, machine learning (ML) approaches. The number of tasks was solved efficiently by ML methods in the papers [12-14]. Thus, the aim of this paper was to predict the dependencies of stress and strain ranges upon number of loading cycles for NiTi SMA utilizing the supervised ML methods.

## 2. Methods

The dependencies of stress range and strain on the number of loading cycles for the four specimens, that were taken from study [15] were predicted by methods of machine learning in the programming platform Orange 3.34.0 [16]. This software allows to build visually the flowcharts and obtain the results in the form of models, numerical data and plots.

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In general, for each of four specimens, two model were built. On the input of each model there were given the dependencies of the respective physical quantity on the number of loading cycles. The number of loading cycles was treated as an independent variable, and the physical quantity was chosen as a dependent variable. To increase the accuracy of modelling results, the dataset was augmented. The data augmentation was performed by interpolating the original experimental data by 1-Dimensional Akima spline. Akima spline is a type of non-smoothing spline that gives good fits to curves where the second derivative is changing fast [17].





For each specimen, the dataset was split into two unequal parts. The training dataset contained 66% of the total dataset. The regression dependencies were built by methods of random forests, neural networks, gradient boosting, support vector machines (SVM), AdaBoost, and k-nearest neigbors methods. Each of the obtained models was checked additionally by k-fold cross-validation method 10 times. Fig. 1 shows the flowchart of one model, built in the programming environment Orange.

## 3. Results and discussion

There was performed the estimation of structural properties of specimens, made of NiTi SMAs. In general, there were tested 4 specimens. The number of specimen, as well as the sample size for stress and strain range versus the number of loading cycles are presented in Table 1.

Table 1. Specimen number and sample sizes for stress and strain ranges versus the number of loading cycles.

specimen #	Sample	e size
	Δε(N)	Δσ(N)
10	1004	1004
13	771	771
16	1059	2049
17	942	942

#### Table 1

Specimen number and sample sizes for stress and strain ranges versus the number of loading cycles

Table 2 presents the results in the form of various prediction errors, such as root mean square error (RMSE) and mean average error (MAE), as well as correlation coefficient  $R^2$  for  $\Delta\epsilon$  and  $\Delta\sigma$ , assessed for specimen #10.

## Table 2

Specimen # 10		Δε			Δσ			
Model	RMSE	MAE	R <sup>2</sup>	RMSE	MAE	R <sup>2</sup>		
Ada Boost	0.014	0.008	1.000	0.776	0.196	0.999		
Gradient Boosting	0.019	0.013	1.000	0.802	0.268	0.999		
kNN	0.019	0.006	1.000	0.636	0.133	1.000		
Neural Network	0.153	0.109	0.987	1.586	1.061	0.997		
Random Forest	0.017	0.008	1.000	0.581	0.163	1.000		
SVM	0.298	0.244	0.950	14.667	13.527	0.744		

Prediction errors and correlation coefficient for  $\Delta \epsilon$  and  $\Delta \sigma$ , built for specimen # 10 using various supervised ML methods

The lowest errors for specimen # 10 were shown by Ada Boost and kNN for  $\Delta \varepsilon$ , and random forest and kNN for  $\Delta \sigma$ . Fig. 2 (a, b, c, d) displays the plots of predicted versus true values of the respective physical quantities, built by the afore-mentioned ML methods.



c) Δσ Random Forest

d) Δσ kNN

**Figure 2**: The predicted versus true values of physical quantities. a) built for  $\Delta \varepsilon$  by means of Ada boost method; b) built for  $\Delta \varepsilon$  by means of kNN method; c) built for  $\Delta \sigma$  using Random Forest method; d) built for  $\Delta \sigma$  using kNN method

As it can seen from Fig. 2, the calculated points are very close to the bisector of the first coordinate angle, that confirms the high prediction accuracy.

The modelling was also performed for the specimen #13.

Table 3 contains the prediction errors and correlation coefficient for  $\Delta \epsilon$  and  $\Delta \sigma$ , estimated for specimen # 13 using various ML methods.

## Table 3

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Specimen # 13		Δε			Δσ	
Model	RMSE	MAE	R <sup>2</sup>	RMSE	MAE	R <sup>2</sup>
Ada Boost	0.071	0.008	0.981	0.607	0.176	1.000
Gradient Boosting	0.071	0.010	0.981	0.619	0.225	1.000
kNN	0.078	0.007	0.977	0.557	0.112	1.000
Neural Network	0.235	0.176	0.796	1.165	0.718	0.998
Random Forest	0.074	0.008	0.980	0.544	0.155	1.000
SVM	0.144	0.080	0.923	13.615	12.797	0.770

Prediction errors and correlation coefficient for  $\Delta\epsilon$  and  $\Delta\sigma$ , built for specimen # 13 using various supervised ML methods

For this particular specimen, the lowest errors were obtained by employing Ada Boost and kNN for  $\Delta \epsilon$ , and random forest and kNN for  $\Delta \sigma$ .

The plots of predicted versus true values of the respective physical quantities, built by the aforementioned ML methods for specimen # 13 can be seen on Fig 3 (a, b, c, d).



**Figure 3**: The predicted versus true values of physical quantities for specimen # 13 a) built for  $\Delta \epsilon$  by means of Ada boost method; b) built for  $\Delta \epsilon$  by means of kNN method; c) built for  $\Delta \sigma$  using Random Forest method; d) built for  $\Delta \sigma$  using kNN method

Table 4 contains the forecast errors and correlation coefficient for  $\Delta \epsilon$  and  $\Delta \sigma$ , built for specimen # 16 using several supervised ML methods.

## Table 4

Prediction errors and correlation coefficient for  $\Delta\epsilon$  and  $\Delta\sigma$ , built for specimen # 16 using various supervised ML methods

Specimen # 16	Δε			Δσ		
Model	RMSE	MAE	R <sup>2</sup>	RMSE	MAE	R <sup>2</sup>

Ada Boost	0.016	0.001	0.971	0.150	0.040	1.000
Gradient Boosting	0.016	0.002	0.971	0.174	0.078	1.000
kNN	0.016	0.001	0.971	0.099	0.023	1.000
Neural Network	0.041	0.025	0.815	0.439	0.257	0.999
Random Forest	0.018	0.002	0.964	0.115	0.033	1.000
SVM	0.077	0.067	0.343	12.133	11.186	0.426

For the specimen # 16, the lowest errors were obtained by employing Ada Boost and kNN for  $\Delta\epsilon$ , and random forest and kNN for  $\Delta\sigma$ .

Table 5 presents the errors and correlation coefficient for  $\Delta\epsilon$  and  $\Delta\sigma$ , obtained for specimen # 17 by means of different ML methods.

#### Table 5

Prediction errors and correlation coefficient for  $\Delta \epsilon$  and  $\Delta \sigma$ , built for specimen # 17 using various supervised ML methods.

Specimen # 17		Δε			Δσ	
Model	RMSE	MAE	R <sup>2</sup>	RMSE	MAE	R <sup>2</sup>
Ada Boost	0.061	0.005	0.961	5.550	0.467	0.866
Gradient Boosting	0.061	0.006	0.961	5.542	0.498	0.867
kNN	0.052	0.004	0.971	4.419	0.316	0.915
Neural Network	0.186	0.085	0.630	5.660	1.115	0.861
Random Forest	0.058	0.005	0.964	3.896	0.339	0.934
SVM	0.152	0.092	0.751	10.815	8.849	0.492

For the specimen #17, the lowest errors were obtained by Random Forest and kNN for  $\Delta \varepsilon$  and  $\Delta \sigma$ .

## 4. Conclusions

There were predicted the structural properties of pseudoelastic NiTi SMA, namely, the dependencies of stress and strain range upon the number of loading cycles, by employing the methods of supervised learning methods. The predicted versus true values of those two physical quantities were built. They are very close to the bisector of the first coordinate angle, which confirms high prediction accuracy. The best results in terms of RMSE and MSE were shown by Ada Boost and kNN for  $\Delta \varepsilon$ , and by Random forest and kNN for  $\Delta \sigma$ . It can be further concluded, that the methods of supervised ML can efficiently predict the afore-mentioned dependencies, and are the promising method to solve such kinds of tasks.

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