

# A New Method to Predict the Mechanical Behavior for a Family of Composite Materials

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## Abstract

This paper introduces a method to develop a common model based on machine learning (ML) that predicts the mechanical behavior of a family with three composite materials. The latter are structures composed of the same carbon fiber and different matrices. The developed algorithms predict the stress given the strain value and eight physical parameters of the matrix. Creating a prediction algorithm (PA) for each composite alongside its training dataset is the straightforward solution. First, the paper develops three separate regression models that model the composite family together. As a main contribution, a model conversion is achieved, turning the set of individual regression models into a single model representing the entire family. This model conversion is advantageous because the training dataset of the family model is much smaller than the combined datasets of the three models. This reduction is possible because the family has a common “feature” that defines the family: the same Carbon Fiber. According to our knowledge, this research topic has not been addressed in the existing literature. An iterative procedure develops regression models for the entire family. For the composites family, the models are trained and tested using data sets generated by a high-performance simulation software. Complex design sessions in MATLAB, which have used Multiple Linear Regression, Support Vector Machines, Decision Trees, Regression Neural Networks, and Gaussian Process Regression, have identified effective PAs. The selection is based on the accuracy of the prediction, mainly indicated by Root Mean Square Error. A family regression model runs 60 - 70 times faster than the simulation software. This helps it work more efficiently and be integrated more easily into an optimization or design program.

## Keywords

Composite Materials Modeling, Regression Models, Machine Learning, Simulation

## 1. Introduction

This paper covers a specific activity of a research project concerning the usage of composite material for the fabrication of hydrogen storage vessels. The scientific actuality of this topic is largely described in many papers, for example [1]. This work addresses an original method for predicting the mechanical properties of a specific family of three composite materials. The method's outcome is an ML prediction algorithm common for the entire family, along with a reduced training dataset. The novelty is an efficient model conversion: transforming the set of individual material models into a single model representing the entire family. According to our knowledge, this topic has never been explored in the literature. The common feature that defines the family, which in our case is the use of the same carbon fiber, is used to reduce the training dataset in comparison with the union of the group's datasets. The family of the three composite is used as an illustrative example; in principle, the method works for any group of objects sharing a common "feature" that could create redundancy in datasets.

The project mentioned above addresses the mechanical behaviour's prediction for composite materials in two cases:

- Composite laminates with various fibers are already presented in [2].
- Composite materials, such as fiber and matrix structures, are the topic of this presentation.

The composite materials' models are developed within two scientific contexts:

- The composite materials science involves mechanical, physical, and chemical knowledge working together to achieve models. Finite element numerical integration is used to construct these models.
- Machine learning algorithms are used to predict the mechanical behaviour of composite materials [3] based on data generated through physical tests or precise simulation campaigns.

The work within the current activity of the project led us to develop ML prediction algorithms for a doubly reinforced composite made of carbon fiber (CF)-reinforced PA12 or another polyamide (PA6, PA11), doped with carbon nanotubes. To avoid confusion with the prediction algorithm (PA), the three composites are labeled as CF/6, CF/12, and CF/11. For example, the material CF/6 consists of carbon fiber and polyamide 6.

For any composite material of this kind, we are interested in describing the prediction of the stress value as a function,

$$\text{stress} = f(\text{strain, other physical parameters}). \quad (1)$$

The function  $f$  can be a regression function, meaning that a statistical model will provide the stress values. ML can define this function implicitly or explicitly.

Datasets for the training and test phases are needed to develop ML prediction algorithms. The specialized finite element simulator DIGIMAT-VA was used to analyze the stress-strain relationships for a family of three materials. From this simulator, datasets were extracted using export files, which were used for this

research.

A usual approach is to develop independently three PAs for the three materials, each with its own training dataset, as if they didn't have the CF in common. Hence, we can not take advantage of the common feature. However, the three materials share a "feature" in their mechanical behavior that comes from the common CF. The unique chance to highlight and take advantage of this common behavior is to develop a common regression model [4]-[8] for the entire family. This is the first idea that groups all composite materials into a family model (a PA is an input-output model, in the broad sense of the word):

1) *A single ML prediction algorithm can be created as a joint prediction algorithm that predicts stress values for the entire family all at once.*

A first approach would be to consider the training dataset for this algorithm as the union of datasets corresponding to all composite materials. But this option still does not take advantage of the common feature. The materials' behavior results from the combination of two factors: the influence of the CF and the influence of the matrix. The training dataset is the numerical expression of the material's behavior. In the case of three separate regression models, the CF's influence on the training dataset for a specific material has no impact on the other two regression models. However, for this first joint PA, which models the composites family, the CF's influence on the training dataset appears to be "repeated". It creates a certain redundancy in the training data points. The possibility that appears now to take advantage of this common "feature" is to eliminate the redundancy in the training data points for the joint PA. The reduced data set size is the mentioned advantage of using the common "feature". This is the second idea that could lead to a reduced training dataset for the family model:

2) *Due to the common "feature", a method that eliminates the redundancy in the training data points will reduce the training data size for the joint PA.*

The two ideas form the rationale behind the original method for predicting the mechanical behavior of a family of composite materials. However, these ideas were still hypotheses at the beginning of our work because the reasoning connecting them relies on intuitive aspects from two different areas: the structure of composite materials and their PAs' numerical training data. In the following sections, the two hypotheses will be validated by constructing a joint PA for the family with a reduced training dataset.

In this presentation, we examine reducing the training dataset for the joint PA, considering that CF/6 and CF/12 provide their original datasets. As a work hypothesis, CF/11 contributes only a few data points to the joint model. In other words, besides the two original datasets, there exists a reduced set of data points characterizing a specific material (e.g., CF/11), for training the joint ML prediction algorithm, ensuring good accuracy for all three materials.

Shared-structure models in multi-task regression utilize similarities among related tasks to improve prediction accuracy and efficiency by sharing parameters and learning from multiple tasks at the same time. Instead of training separate

models for each task, these models share parts of the model, like layers in a deep neural network, across different tasks. The related regression tasks refer to the same object (entity or system). It is about a “multi-task” problem involving the same object. In the proposed method, we have a family of objects (entities)—in our case, the composite materials are different objects from the perspective of materials science. The goal is to solve a single task, a regression model for the entire family, that is more efficient than the trivial solution described before. So, this time we have a single regression task that must be constructed for a multi-object target.

Rather than building a new model from scratch, transfer learning uses a pre-trained model as a starting point. In our study, transfer learning is not involved; constructing individual regression models for the three materials only validates the existing training datasets, but they are not used further for building the family model.

The main objective of this paper is to present this method and an iterative procedure that implements it. The solution is not unique and can be adjusted according to the desired accuracy. The key factor in the accuracy improvement is gradually increasing the number of data points (e.g., for CF/11) added to the training set.

The developer conducts multiple design sessions where basic ML models, such as Multiple Linear Regression, Support Vector Machines, Decision Trees, Gaussian Process Regression, and RNN, generate regression algorithms.

Generally, the simulation of material performance under real-world conditions enables a precision of up to 95% correlation with physical testing results [9]. Simulations integrated in a design application provide high-quality data but take much more time than predictions. That is why replacing simulations with accurate predictions can be a realistic solution for this kind of application.

Integrating Artificial Intelligence, comprising machine learning and deep learning, into composite material science has significantly enhanced the construction of regression algorithms and optimization. The existing literature has emphasized two prominent topics: identifying the material properties and the relationship between different parameters, such as mechanical behaviour.

A few articles about the material properties can be mentioned here because the ML techniques are the same as for mechanical behavior. For example, Vahed *et al.* [10] show how neural networks can improve the prediction of dynamic mechanical properties. In the review [11], the main goal is to examine various machine learning and deep learning techniques used for predicting the mechanical properties of composites. AI accurately predicts the mechanical properties of materials, including strength, stiffness, elasticity, plasticity, ductility, brittleness, toughness, and hardness. This is important in various engineering fields.

Ho *et al.* have demonstrated in [12] that Young’s modulus of polymer composites reinforced with carbon nanotubes can be predicted using ML algorithms. The accuracy surpasses traditional testing methods by about 25%, supporting the development of new materials.

Ensemble machine learning methods for predicting the mechanical properties of carbon fiber reinforced composites are discussed in [13]. They employ various ML models, such as Random Forest, Gradient Boosting, and XGBoost, to examine the effectiveness of multi-stacking learning techniques compared to traditional methods.

In [14], predictions are made by analyzing an image of the material microstructure and using knowledge of the constitutive models for fibers and matrix, without performing physically-based calculations. The ML prediction uses a gradient-boosted tree regression model. The latter delivers the most accurate predictions.

The mechanical properties of carbon fiber composites are predicted using a Convolutional Neural Network—Long and Short-Term Memory in [15]. The predictions are within 5% of the corresponding tensile mechanical experimental results.

In [16], the authors used several ML models: Ridge Regression, Bayesian Ridge Regression, Lasso Regression, K-Nearest Neighbor Regression, CatBoost Regression, Decision Tree Regression, Random Forest Regression, and Support Vector Regression. The ML analysis confirmed that fiber content is the most influential parameter in elasticity ( $E$ ) and strength ( $\sigma$ ). The results show that the K-Nearest Neighbors and CatBoost models provided the closest predictions for  $E$  and  $\sigma$ .

Papers that address the mechanical behaviour of composite materials are also numerous and treat different facets of the problems. Convolutional neural networks combined with principal component analysis can accurately predict stress-strain behaviors from microstructural images of composites [17]. This method has decreased computational time by 40% compared to traditional finite element analysis, offering a fast and scalable tool for material design.

Campbell [18] has highlighted AI's role in predicting the mechanical behavior of composites under different stress conditions.

In [2], ML models for composite laminates with various fiber orientations allow a comparative analysis of these materials. The second topic is an innovative method that utilizes ML models to predict complex behaviors for known or new stratification combinations. These models enable the simulation and prediction of composite performance with unmatched accuracy and efficiency, significantly reducing the time and cost associated with experimental testing. Paper [19] is a review focused on the use of ML techniques in analyzing the mechanical behavior of fiber-reinforced polymers (FRP). The ability to achieve high accuracy, along with lower computational costs after training ML models, makes it a valuable tool for optimization and detailed analysis of laminated FRP.

The ML prediction algorithms developed in [20] [21] can “learn” the behavior of an optimizer (a program that optimizes a structure) that makes a lot of computations. Therefore, it can replace the optimizer, for example, in the optimal design of composite materials. The reader can be interested in the practical techniques used in ML prediction algorithms. They will find all the needed information to follow this work in [6] and [8]. More recent references concerning efficient learning for composite property prediction are [22] [23].

In the sequel, Section 2 presents the materials and methods used in this work. Readers will find answers to several questions: Who generates the datasets for the ML algorithms? What ML models are used to develop prediction algorithms? What are the practical objectives? Subsection 2.2 covers the data preparation, while Subsection 2.3 develops the individual prediction algorithms for CF/6 and CF/12. Section 3 presents the method for developing joint prediction algorithms for the entire materials family. The iterative procedure that implements the method is described using the algorithm Generate Common PA. The results are discussed in Section 4, and the Conclusions section resumes the paper's contribution and future work.

## 2. Materials and Methods

### 2.1. Machine Learning Algorithms for Stress Prediction in Composite Materials

The main goal is to analyze the composite materials' stress versus strain relationships and develop prediction algorithms for the stress value. The prediction algorithms must also take into account the values of other material parameters to differentiate among the composite materials. It is about the three composite materials forming the family that have a common feature, which consists of the same carbon fiber (CF). It is important to clarify several aspects from the outset:

1) Who generates the data sets for the prediction algorithms?

Before constructing the ML algorithms, the specialized finite element simulator DIGIMAT-VA was used to analyze the stress-strain relationships of the three materials. Physical parameters and assessed rupture criteria provided insights into the materials' responses to mechanical loading. The simulation software calculates the stress values for various strain values across undamaged (elastic) and damaged (plastic) zones, excluding the rupture zone.

Datasets were collected in exported files and used for training in this research.

2) What ML prediction algorithms is this work aiming to develop?

ML regression models use imported datasets to train and validate regression algorithms, which are referred to as prediction algorithms later on. The models best suited to our problem—such as Multiple Linear Regression, Support Vector Machines, decision trees, Gaussian Process Regression, and RNN—were used for each prediction algorithm developed in this work. The prediction algorithms are implemented as MATLAB functions and scripts, version R2024a. Based on the strain and other parameter values, this model predicts the stress value much faster than conducting a finite element calculation.

3) What practical objectives does this work aim to achieve?

The main objective is to validate the two hypotheses on which the proposed method relies. At the same time, we propose an iterative procedure for constructing joint PAs with smaller training datasets.

First, it has been confirmed that sufficient data points are available to develop the prediction algorithms for CF/6, CF/12, and CF/11. These PAs are referred to

as ML/6, ML/12, and ML/11. For example, ML/6 is the Machine Learning prediction algorithm for the composite material CF/6, and so on.

Given that the three materials share the same carbon fiber, we investigated whether the predictions for the mechanical behavior of CF/11 can be derived from a joint prediction algorithm for both CF/6 and CF/12; the latter is referred to as ML/6-12. This time, the data points characterizing the three composite materials will include variables reflecting the properties of the matrices. We added a certain number ( $n_{11}$ ) of datapoints characterizing the material CF/11 to the datapoints for CF/6 and CF/12 to generate, after training and testing, a new PA, referred to as ML/6-12-11. We have examined how small  $n_{11}$  can be while still maintaining good accuracy in the predictions for CF/11. The details of our investigations are provided in Section 3.

## 2.2. Data Preparation

The data used to develop the prediction algorithms for the stress-strain relationships of the three composite materials are contained in files obtained from simulations conducted using the software DIGIMAT-VA. The material parameters for carbon fiber and matrices are also available.

Data needed for the training of ML/6, ML/12, and ML/11 are available in tables similar to **Table 1**.

**Table 1.** The first ten lines of the table, with 203 lines for CF/6.

Strain11	Stress11 (MPa)
5e-14	6.0014e-09
0.0005	60.014
0.000 853	102.38
0.001 353	129.17
0.001 853	153.49
0.002 353	175.29
0.002 853	194.54
0.003 353	211.3
0.003 853	225.68
0.004 353	237.84

**Table 1** is sufficient for constructing the PA for the stress-strain relationship corresponding to a load direction. However, the material parameters must be added to the data points to identify the composite material. In this way, there is a possibility of creating a common model for the family further. In addition to the load direction (“LoadD”), eight material parameters are listed in the adjacent columns:

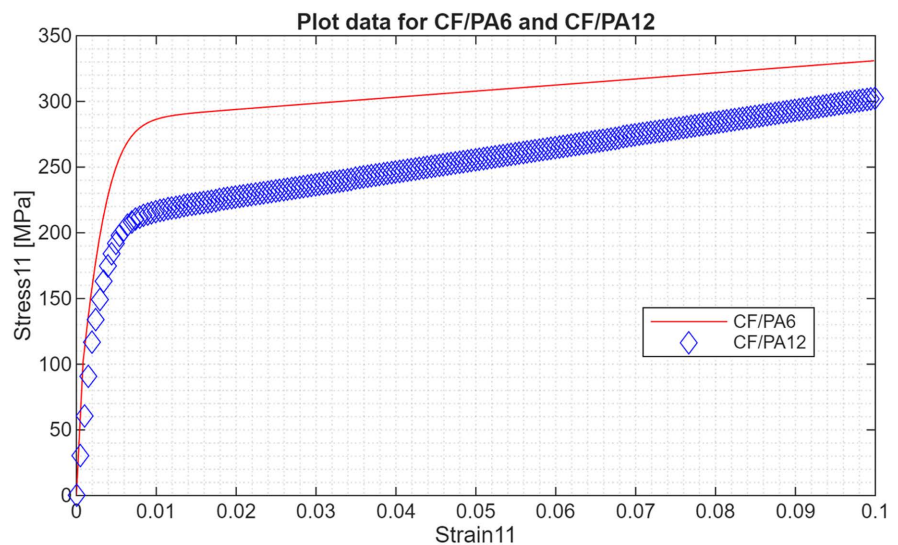
Density (tonne/mm<sup>3</sup>) [20°C - 25°C];  
 Matrix Young Modulus  $E_m$  (MPa);  
 Poisson Ratio, Yield Stress (MPa);  
 Yield Stress (MPa);  
 Hardening Modulus (MPa);  
 Hardening Exponent;  
 Linear Hardening Modulus (MPa);  
 Volume Fraction  $V_f$ .

**Table 2** presents the structure of the dataset for CF/6, which consists of 203 data points and 11 predictors, along with the values of the material parameters required by the joint PA.

**Table 2.** The first five lines of the dataset for CF/6, which consists of 203 data points.

LoadD	Density	$E_m$	Poisson	YieldS	Hm	He	Lhm	$V_f$	Strain11	Stress11
LD11	1.14e-09	3000	0.37	25	3000	0.17	1000	0.6	5e-14	6.0014e-09
LD11	1.14e-09	3000	0.37	25	3000	0.17	1000	0.6	0.0005	60.014
LD11	1.14e-09	3000	0.37	25	3000	0.17	1000	0.6	0.000 853	102.38
LD11	1.14e-09	3000	0.37	25	3000	0.17	1000	0.6	0.001 353	129.17
LD11	1.14e-09	3000	0.37	25	3000	0.17	1000	0.6	0.001 853	153.49

**Figure 1** depicts the relationship between stress and strain as a result of the data in tables like **Table 2**. The elastic and plastic zones are highlighted.



**Figure 1.** Elastic and plastic zones for CF/6 and CF/12.

For data preparation of all PAs involved in the implementation of the proposed method, the following actions are carried out.

- 1) The data imported from the simulator are used to create tables “T6mB,”

“T12mB,” and “T11mB” for the three materials, CF/6, CF/12, and CF/11, respectively.

2) The matrix “Mat6” is the image of the table “T6mB” after eliminating the first 2 columns.

3) “Mat6s” is a selection of Mat6’s lines (one-third of its lines).

4) The matrix “Mat6b” is created by adding three perturbed lines for each line of “Mat6s.” The perturbation ranges uniformly from  $-2\%$  to  $+2\%$  of the values in “Mat6s”.

5) - 7) Perform actions similar to steps 2 through 4, but considering the data related to CF/12.

8) Create the matrix “Mat11b” using the first three lines of “T11mB” and adding nine perturbed lines as before.

9) Create “Mat6\_12\_11” by concatenating the lines from “Mat6b”, “Mat12b”, and “Mat11b”.

10) Transform “Mat6\_12\_11” into a table called “Tab6\_12\_11.”

11) Create the tables “Tab6\_12\_11train” and “Tab6\_12\_11test” using 75% of the datapoints from “Tab6\_12\_11” for training and 25% for testing.

12) Save the tables “Tab6\_12\_11”, “Tab6\_12\_11train”, and “Tab6\_12\_11test” to a workspace file.

The reader can review the “[TMSCE supplementary](#)” folder attached to this article for details on implementing these activities.

Activity 8 results in a minimal contribution of CF/11 to the family exploratory model developed in section 3.3. A more consistent contribution of CF/11 is addressed through the iterative procedure described in section 3.4.

The data-generating process must utilize a probability distribution to satisfy the assumption of independent and identically distributed samples. We have acknowledged that uniformly distributed noise perturbs the data points. This adjustment, considered at points 4 and 8, enhances parameter diversity and improves the generalization.

**Table 3** summarizes the size of the datasets used to develop the PAs throughout this work.

**Table 3.** Dataset size.

	Number of Data Points		
	Training	Validation	Testing
Single materials: CF/6, CF/12, CF11	276	5-fold cross-validation	40 - 80
Joint model ML/6-12 for CF/6 and CF/12	423	5-fold cross-validation	141
The family model ML/6-12-11 for CF/6, CF/12, and CF/11 and $n_{11} = 56$	470	5-fold cross-validation	82; 46
The family model ML/6-12-11 for $n_{11} \in [19, 92]$	433...506	5-fold cross-validation	144...168

The last two lines of **Table 3** cover the iterative procedure described in Section 3.4

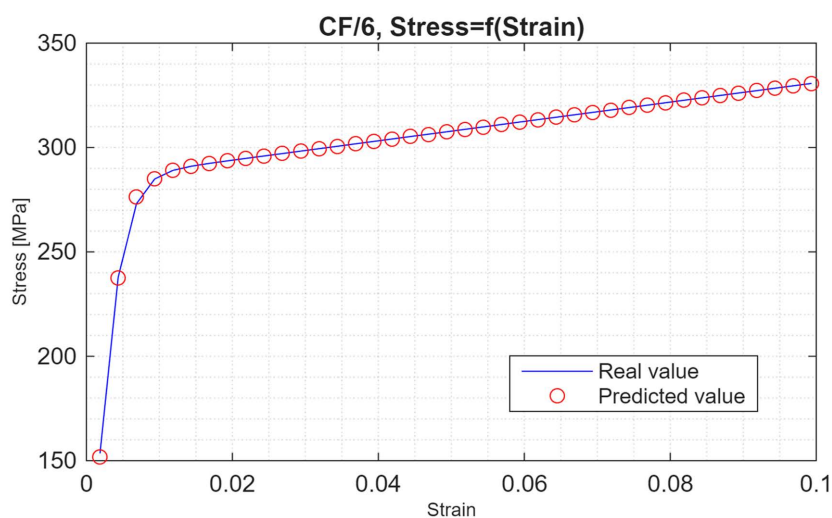
### 2.3. ML Models Used to Train Prediction Algorithms

The models best suited to our problem were already listed earlier. For each PA developed in this work, all five models are used to train the algorithm, and the models' accuracy is compared with each other. Finally, the PA with the best accuracy is selected. This procedure will be referred to as the Design Session. Regression Neural Networks and Gaussian Process Regression are the ML models that produced the best results each time. They were better suited for our problem, both for single and joint regression algorithms. The quality criterion was the accuracy of the predictions, mainly expressed by the value of RMSE (root mean square error) between the real and the predicted stress values.

### 2.4. ML Prediction Algorithms for a Single Composite Material

Design Sessions have identified the most accurate models for the stress-strain relationships of both CF/6 and CF/12. As an example, the ML/6 is the result of a trained ML model, which is an RNN. For ML/12, an RNN was also developed.

**Figure 2** draws the curves of the real and predicted values of the stress using ML/6.



**Figure 2.** Stress versus strain functions: real and predicted values.

**Figure 2** demonstrates that the ML/6 model's predictions are highly accurate. Similar results are obtained for ML/12 and ML/11.

## 3. Implementation and Results

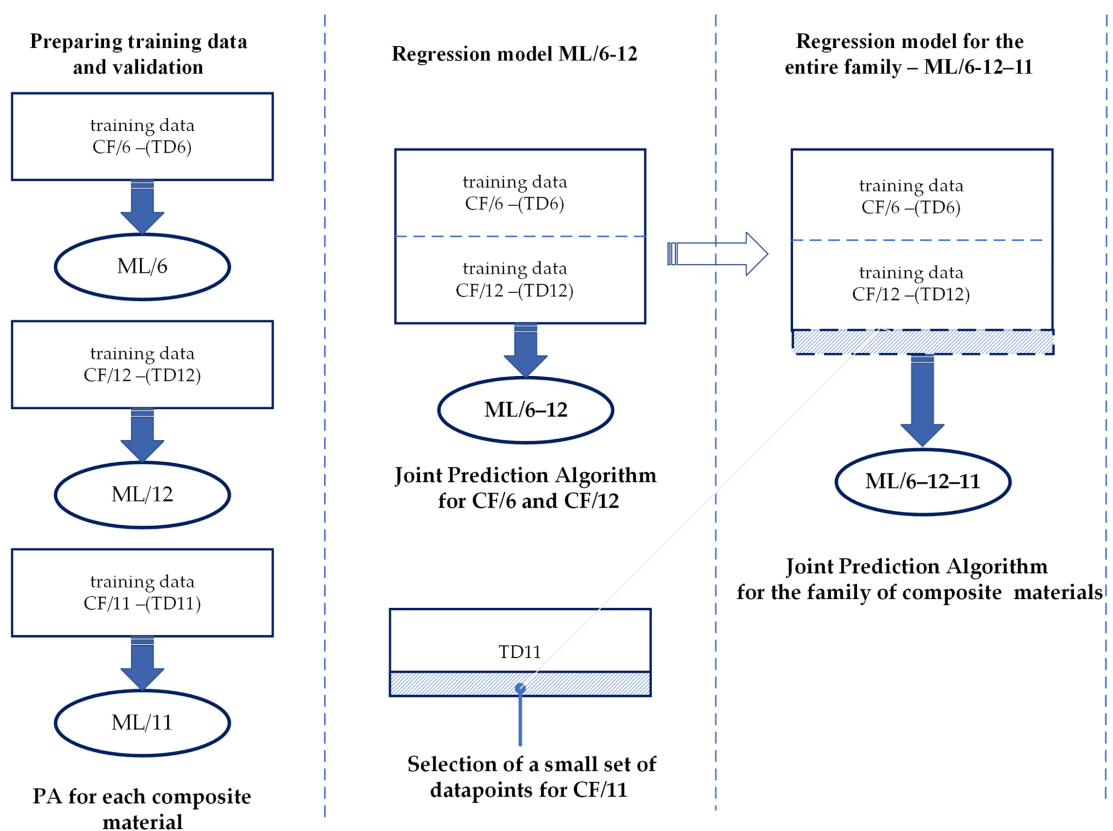
### 3.1. General Approach to Constructing a Joint PA for CF/6, CF/12, and CF/11

The previous sections have shown that prediction algorithms can be effectively

developed for the composite materials CF/6 and CF/12. Since the composite material CF/11 uses the same fiber as the other two materials, we will explore the following approach to predict the stress for CF/11:

- We shall construct a single prediction algorithm characterizing both composite materials simultaneously, CF/6 and CF/12. This model will be referred to as ML/6-12.
- We assume that the composite material CF/11 follows the ML/6-12 model since it uses the same CF. We will test whether this model applies to the behavior of CF/11 and if the predictions align with the actual stress values. If the predictions are inaccurate, we will add a specific number of data points (n11) that characterize the CF/11 material.

The phases of constructing the common model are presented in **Figure 3**, which also presents the names of the regression models.

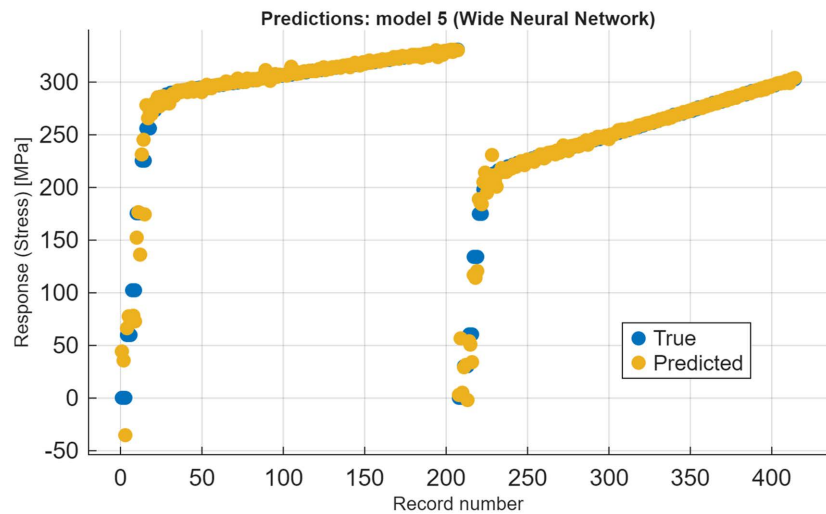


**Figure 3.** Construction phases of the common model for the entire family of composite materials.

### 3.2. The Model ML/6-12

This section develops a regression model ML/6-12 that simultaneously provides accurate predictions for both materials CF/6 and CF/12. It is trained using the combined training datasets from ML/6 and ML/12.

A design session has generated an RNN model (model 5—a wide NN). Using the model ML/6-12, the data from **Figure 4** and **Table A1** are generated.



**Figure 4.** Actual and predicted values obtained using ML/6-12, which is a wide NN.

The predicted values for the testing data are shown in Appendix A, **Table A1**, column “StressPred”. The stress values for CF/6 and CF/12 are accurately predicted for all data points, as demonstrated by **Figure 4**, **Table A1**, and the statistics:

- Size of training data: 423 observations; validation: 5-fold cross-validation.
- $\text{vrms} = 3.24$  (the RMSE using the test data set during the training procedure),
- $R^2 = 1$ ;  $\text{MAE} = 1.3261$  (the Mean Absolute Error in test during the training procedure;
- $\text{RMSE}_{\text{Valid}} = 6.7645$  (the RMSE after training using a test dataset composed of unseen data points).

We used this model, ML/6-12, for 50 test data points characterizing CF/11. The predictions are inaccurate. Moreover, by repeating the call for predictions, the algorithm returns other values, which means it has random behaviour when treating these data points.

Although the carbon fiber is the same, the matrix has different parameters. The model ML/6-12 can only make predictions based on the data it was trained on, which is a logical fact. In the following subsections, we propose a method to leverage the fact that the three materials share the same carbon fiber.

### 3.3. An Exploratory ML/6-12-11 Model Trained with a Very Small $n_{11}$

This subsection aims to extend the applicability of ML/6-12 by incorporating additional data points regarding CF/11 at the lower end of the strain range. These data points near the null strain can impose fixed points through which the function  $f$  will pass. In other words, they could eliminate an indefinite tendency of the predictions. We expect the strain-stress function to pass through several points in the lower end of the strain range.

Initially, we added a very small number of data points ( $n_{11} = 12$ ) related to

CF/11 to obtain a set of 423 data points describing CF/6 and CF/12. The new model, ML/6-12-11, will recognize CF/6 and CF/12 just like the ML/6-12 model does.

After examining other ML models in this new context, a better model is constructed using GPR (Gaussian Process Regression), which generates Model 7 (we kept the notation used in the project), whose hyperparameters are given in Appendix B.

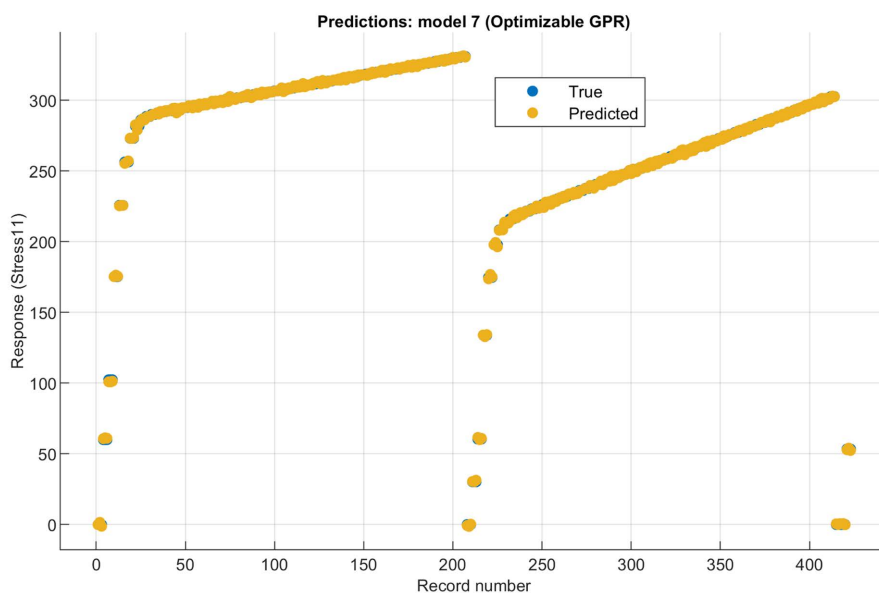
The training and the validation give very good values for the root mean square error. The statistics are:

- Size of training data: 423 observations; validation: 5-fold cross-validation.
- $\text{vrms} = 0.74923$  (the RMSE using the test data set during the training procedure),
- $R^2 = 1$ ;  $\text{MAE} = 0.2979$  (the Mean Absolute Error in test during the training procedure);
- $\text{RMSE}_{\text{Valid}} = 0.38761$  (the RMSE after training using a test dataset composed of unseen data points).

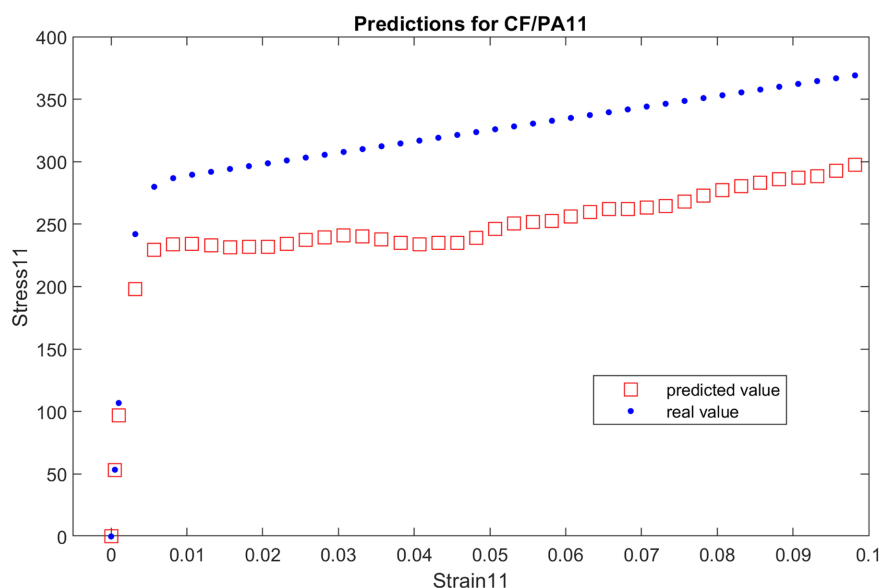
The predictions made by Model 7 are described in **Figure 5** and **Table A2** (Appendix B).

The algorithm ML/6-12-11 implemented by Model 7 provides improved predictions for CF/6, CF/12, and the few data points related to CF/11. But, predictions for datapoints related to CF/11 and not in the training set are inaccurate. As illustrated in **Figure 6**, these predictions indicate a trend, but they lack accuracy in predicting stress over the entire strain range.

Consequently, only a few data points regarding CF/11 at the lower end of the strain range are not enough to make the algorithm ML/6-12-11 able to predict the stress values for CF/11 accurately.



**Figure 5.** Actual and predicted values were obtained using a joint PA, ML/6-12-11, with a very small  $n_{11}$ .



**Figure 6.** The model 7 inaccurately predicts CF/11, but it does show a tendency.

### 3.4. An Iterative Procedure for Developing Prediction Algorithms for the Entire Family of Composite Materials

The conclusion of the previous section indicates that more data points related to CF/11 are necessary to cover a broader range of strain values. This will help the algorithm “learn” more effectively from evenly distributed strain values over the strain’s range.

Through an iterative procedure, new joint PAs are developed for the entire family. They are all designated as ML/6-12-11. The **Generate Common PA** algorithm implements this procedure. For the third composite, the developer selects a variable number  $n_{11}$  of data points. The complete training dataset is formed by combining the dataset for ML/6-12 with the  $n_{11}$  data points. The dataset for ML/6-12 is already set; it contains  $n_6 + n_{12}$  data points. After training, the accuracy is evaluated using the same test datasets containing unseen data points for CF/11. The PA’s accuracy improves as the number  $n_{11}$  increases. The iterative process stops when the developer considers that a balance between accuracy and efficiency in using data points for CF/11 has been achieved.

The efficiency of using data points for CF/11 is considered inversely proportional to the ratio  $n_{11} / (n_6 + n_{12} + n_{11})$ , where the denominator represents the total size of the training dataset. The efficiency of using data points for CF/11 decreases as  $n_{11}$  grows. When searching for good values of  $n_{11}$ , this ratio must be less than a superior bound “ $p$ ”.

Our problem has no unique solution. Variable  $n_{11}$  may have different values; the resulting PAs have varying accuracy in predicting CF/11’s stress values. The Generate Common PA algorithm terminates with a solution that depends on the developer’s choices, including the desired accuracy level for predicting stress values and the value of  $n_{11}$ .

The iterative process begins with  $n_{11}$  set to 0 and gradually increases its value, meaning the efficiency decreases while the accuracy of the predictions improves. A test dataset, TD, consisting only of unseen data points related to the CF/11 material, is also prepared. This test dataset will be used in step #6 to allow the comparison among RMSE values.

To produce “good” solutions,  $n_{11}$  must satisfy the constraint specified in step #2—for the “while” structure. The choice of the constant  $p$ 's value is at the developer's latitude (In this work,  $p = 0.2$ ).

Step #3 states that the  $n_{11}$  data points must be evenly spread across the entire strain range. This can be done, for example, by dividing the strain range, which in our case is  $[0, 0.1]$ , into equal intervals and selecting data points whose strain values fall into each interval.

Steps #3, #5, and #8 depend entirely on the developer's choices.

#### ALGORITHM: Generate Common PA

---

/\*Joint prediction algorithms for the entire family are developed\*/

---

Input Data: The training data used for the model ML/6-12  
The complete training data used for the model ML/11

---

Output: The solution considered the best by the developer:  
The regression ML/6-12-11 represented by an object that can be used subsequently.

---

**begin**

---

Initializations:

Generate a test dataset (TD) consisting only of unseen data points related to the CF/11

1  $n_{11} \leftarrow n_{11_0}$ ; /\*Initialize  $n_{11}$ , the number of datapoints concerning CF/11, added to the general dataset\*/  
 $stop \leftarrow 0$ ; /\*Stops the iterative procedure when it equals 1\*/

---

2 **while** ( $n_{11} / (n_6 + n_{12} + n_{11}) \leq p$  **and**  $stop = 0$ ) **do**

---

3 Select  $n_{11}$  data points related to the material CF/11, ensuring they are evenly distributed across the strain range

---

4 Prepare a new dataset for training a new PA, ML/6-12-11, by adding the new  $n_{11}$  datapoints

---

5 Conduct a Developing Session aimed at constructing a new prediction algorithm for ML/6-12-11

---

6 Test the prediction accuracy of the new algorithm ML/6-12-11 using TD

---

7 Save the statistics and plots

---

8 **if** (ML/6-12-11 has a satisfying accuracy), **then**  $stop \leftarrow 1$   
**else** {Select an increment  $\Delta n$ ;  $n_{11} \leftarrow n_{11} + \Delta n$ ;}  
9 **end** /\*while\*/

---

**end**

---

The value  $n_{11_0}$  is entirely at the latitude of the developer. The latter is interested in finding a small value for  $n_{11}$ , meaning that the efficiency is good. In our case, the exploratory model showed that  $n_{11} = 12$  is not enough. The data points cover

the strain range using 276 values. Considering these values with a step of 15 (1, 16, 31, ...), this corresponds to  $n_{10} = 19$ .

The value  $\Delta n$  is chosen subjectively by the developer at each step of the iterative process. Based on the accuracy achieved at the current step, the developer will determine the next value of  $n_{11}$ .

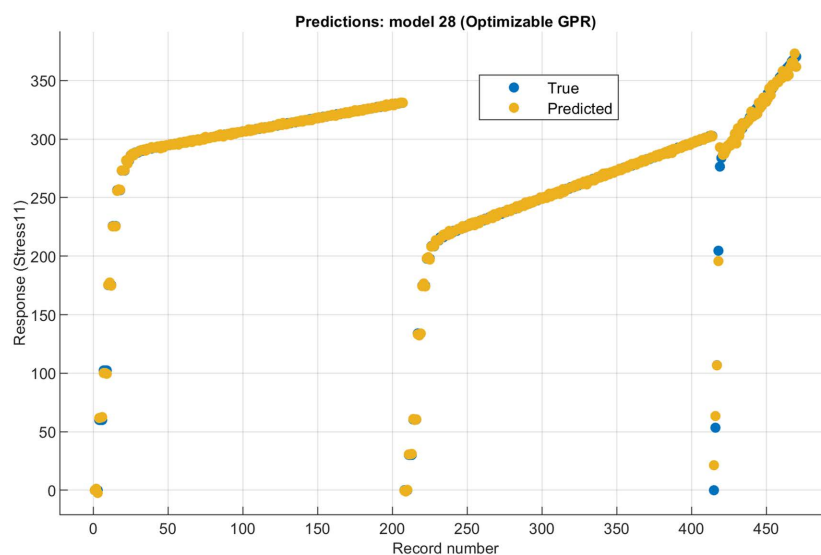
In our study, the value  $p = 0.2$  corresponds to  $n_{11} = (n_6 + n_{12}) / 4$ . Beyond this value, the efficiency of using the family model is questionable. But the value  $p$  can be set subjectively.

Carrying out Generate Common PA, more ML/6-12-11 algorithms are generated by the GPR model. Different values of  $n_{11}$  generate different training datasets. The GPR model (an optimizable version) is generated after training a series of different PAs. From this series, four PAs—mdlGPR26, mdlGPR27, mdlGPR28, and mdlGPR29—are presented below (we kept the notations from our implementation). The four models are derived from training the basic GPR model with different datasets; the data points for CF/6 and CF/12 are identical, only  $n_{11}$  increases.

The mdlGPR28 algorithm is developed by adding  $n_{11} = 56$  data points (its hyperparameters are given in Appendix C). For this PA, **Figure 7** shows the predicted and actual stress values for all the records.

The statistics are:

- GPR, Bayesian optimization,
- Size of training data: 470 observations; validation: 5-fold cross-validation.
- $\text{vrms} = 0.914\ 45$  (the RMSE using the test data set during the training procedure),
- $R^2 = 1$ ;  $\text{MAE} = 0.599\ 45$  (the Mean Absolute Error in test during the training procedure;
- $\text{RMSE}_{\text{Valid}} = 1.970$  (the RMSE after training using a test dataset composed of unseen data points).



**Figure 7.** The ML/6-12-11 algorithm implemented with mdlGPR28: predicted and real values for all the records.

To illustrate the accuracy evolution during the iterative procedure, the predictions made by the four PAs are shown in **Figure 8**. Consequently, the efficiency of using data points for CF/11, as we have defined it, decreases. In contrast, the prediction accuracy of the four models improves, as shown in **Table 4**. A special test dataset is used to determine predictions for all PAs generated in the iterative procedure. Therefore, a comparison can be made among models using the RMSE value.

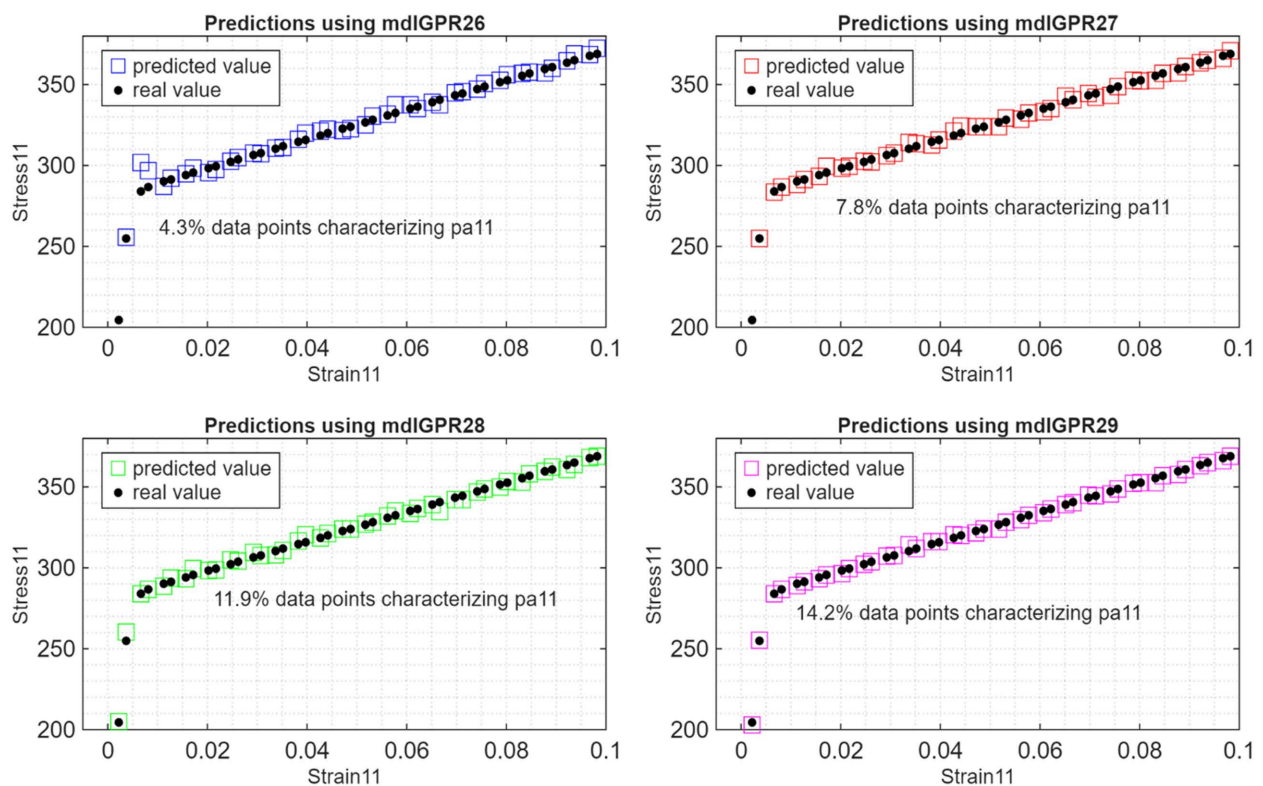
**Table 4.** Efficiency and accuracy of the four models.

Model	mdlGPR26	mdlGPR27	mdlGPR28	mdlGPR29
$n_{11} / (n_6 + n_{12} + n_{11})$	4.3%	7.8%	11.9%	14.2%
RMSE	6.001	2.278	1.970	1.107

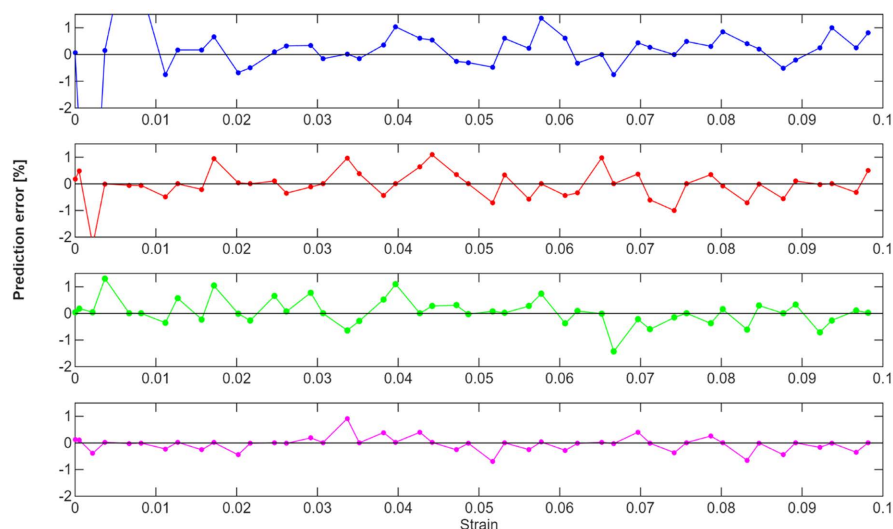
The prediction error also offers insight into the accuracy of the predictions, which is not purely statistical. It is defined by the following ratio expressed in [%]:

$$(\text{predicted stress value} - \text{actual stress value}) / \text{stress range}.$$

For our composite materials, the stress range is 400 MPa. **Figure 9** shows the prediction errors for the test dataset. Only the error values within the interval  $[-2, 1]$ % are displayed to simplify model comparisons. The last three PAs generate small prediction errors within the interval  $[-1, 1]$ %.



**Figure 8.** Accuracy evolution in the iterative process.



**Figure 9.** Prediction errors of the PAs generated in the iterative process.

The accuracy of the model mdlGPR28 is very high, so it could be the solution to our goal of building a PA with a reduced training dataset. **Table A3** (Appendix C) gives numerical results that are even more convincing than **Figure 8**.

Obviously, it is not surprising that accuracy improves and errors decrease as the training datasets grow. But the proposed algorithm allows developers to solve the problem gradually in an interactive way. It is up to them when to stop the procedure and choose a solution based on their subjective judgment (considering, eventually, other criteria).

## 4. Discussion

### Modeling a family of materials.

Throughout this paper, the term model is often used as in “machine learning model” to refer to a basic ML model (such as a regression model like Regression Neuronal Network, or Support Vector Machine) whose parameters must be set through training. In the sequel, the word “model” will be used directly in its common scientific sense, namely, the result of the mathematical modeling.

As mentioned in the Introduction section, the function  $f$  in Equation (1) can be a regression function, meaning that a statistical model will provide the prediction for the stress value. ML can define this function explicitly (e.g., multilinear regression) or implicitly (e.g., a Regressive Neural Network).

Because tensile tests on composite materials are the main contributors in supplying data on the mechanical behaviour, Equation (1) is naturally applied to each material; therefore, we use a regression model for each member of the family. A regression model is a non-deterministic mathematical model. As an initial approach, predicting stress means constructing three different models (in the sense of mathematical models).

From the point of view of modeling the composite family, the context is characterized by the following aspects:

- A model was developed for each member of the composite family.
- The composites' models have static (non-dynamic) character, and are input-output models. The stress is the output, and the inputs are the strain and the other eight parameters.
- Finally, the family is modeled by a single model representing simultaneously the three materials.
- At the implementation level, this mathematical model is represented by one of the ML/6-12-11 algorithms (implemented by a method within an object belonging to a class).
- The family model is more efficient in using the resources (like memory; it needs fewer datapoints to be trained).

Remark: Besides the modeling of individual composites, the work presented in this paper achieved a model conversion: turning the set of individual material models into a single model representing the entire family.

Besides the prediction of stress or other parameters, a compact family model could help in other applications, such as materials design, optimization, etc.

#### **The GPR outperforms the other ML models.**

Following our experience in using the regression models, the RNN in almost all cases supplies very accurate prediction algorithms. Therefore, we expect that an RNN will be one of the top two most accurate ML models, if not the most accurate. The price to pay is generally the size of the model, which is among the greatest.

In this work, the models presented in sections 3.3 and 3.3 confirm this expectation, but in each case, the best prediction algorithm is derived from the Gaussian Process Regression. One might wonder if there is a particular reason why the GPR algorithm performs better than the RNN algorithm. In the authors' opinion, the reason is related to the particular shape of the curves that the ML model needs to "learn". Each joint model of the three composite materials has the plot of the stress-strain function formed by three curves, corresponding to the three composite materials. Two nearly linear segments essentially form each of the three curves corresponding to the elastic and plastic zones. On the other hand, the joint distribution of latent variables in the GPR model is close to a linear regression model (all the kernels form a matrix that plays the role of the covariance function) [24]. This may be the reason why the six "linear" segments can be more efficiently "learned" by the GPR model.

#### **Other aspects.**

Finally, with 11% of data points related to CF/11 included in the training set, we obtained very good accuracy, as the statistics prove. This is not the lower bound of  $n_{11}$ . A smaller number  $n_{11}$  may reduce the prediction algorithm's accuracy, but it will still provide acceptable stress predictions required by the current application.

The applicability limitations of the proposed prediction algorithms are limited. First, they only cover the elastic (linear) and plastic (nonlinear) zones. There is another nonlinear zone—the rupture zone—where the material is damaged. Our

algorithms do not address this zone because it is not the focus of ML at this stage of the project.

The ranges of the strain and stress values are entirely covered by the algorithms (in datasets and predictions). They are specific to the three composite materials working in both zones (which are known for each material and specified before constructing the algorithms). For the same strain value, the three materials have different stress responses. That is why variables characterizing the matrices must be included in datasets so that the material can be identified and the stress accurately predicted for each.

In the context of our work, the following question can be considered: if we use a new polyamide instead of PA11, will the proposed method work for all three materials? The answer is yes, the unique difference is the use of a new polyamide dataset. The same perspective applies whenever another family of materials is involved. Only the material with a small number of data points needs to be specified. Our approach generally applies in this context, but the efficiency of the overall prediction algorithm may differ (the ratio between the small number and the total number of datapoints can vary).

The regression models developed in this study depend on the quality of data characterizing the mechanical behavior of the family of composite materials. In our case, the datasets were provided by the DIGIMAT simulator, which is well-known for producing simulation data that matches that obtained from physical tests (see, for example, [2]). Physical tensile tests have been conducted, and their results have been used to calibrate the simulator DIGIMAT-VA, which provides a very high precision. The method to construct a regression model for the family of composite materials can utilize datasets from another acceptable simulator or only physical tests, even if the latter is an expensive approach. That is why the proposed method can also be applied in other scenarios where a group of objects shares a common feature that cannot be measured. Of course, the accuracy of results depends on the quality of the dataset provided as input.

As the simulations proved, a prediction algorithm runs 60 - 70 times faster than the simulation software. This fact helps it integrate and work more efficiently within an optimization program, especially when a joint model for the entire family is available.

## 5. Conclusions

In this work, several joint models of the composite family have been developed. Each of them uses a smaller training dataset. Therefore, the two ideas behind the proposed method for constructing a family model have been confirmed.

The main contribution of this work is the proposed method to develop a common model for the entire family of composite materials. Essentially, this method achieves a model conversion: the set of individual material models is transformed into a single model representing the entire family. The family model is a regression model that allows simultaneously predict the stress for each material as in Equation (1).

The following aspects highlight the importance of this original method:

- It can be adapted to any number of composite materials, not only three.
- It can be adapted to allow predicting other parameters when an equation similar to (1) is available.
- The smaller number of data points related to one material can reduce the cost and simulation time when preparing data for prediction algorithms.
- Family models have a general character because they can be applied to any family of objects, not only to composite materials, as long as the common feature defining the family is related to the training dataset.
- Family models are more easily integrated into optimization and other types of programs: a previous selection of an individual model is no longer necessary.

The second contribution of our work is the iterative procedure itself, which helps the developer in building the family regression models (ML/6-12-11) and finding a balance between accuracy and efficiency. This iterative procedure is implemented using the algorithm **Generate Common PA**.

Because the simulated data is highly reliable, further studies and implementations within the current project will require a reduced set of tensile tests.

The authors envisage that the prediction algorithms developed in this project will be used to solve optimization problems related to composite laminates with various fiber orientations. Composite materials can consist of multiple layers with different fiber directions. Identifying the orientations that maximize the resilience of the composite is a problem with high computational complexity. A module capable of quickly calculating specific parameters is therefore desirable. ML prediction models can provide very fast, accurate results, 60 - 70 times faster than DIGIMAT simulations. A realistic approach is to find quasi-optimal solutions using metaheuristic optimization techniques like Genetic Algorithms or Particle Swarm Optimization.

Whether focused on composite materials or not, readers interested in developing prediction algorithms can find support in our work for their applications. They can access the MATLAB scripts, functions, and other files related to this work, which are available in the "[JMSCE supplementary](#)" folder attached to this paper.

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## Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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## Appendix A

The reader can open the archive "[TMSCE supplementary](#)" and read the document "Guide for using the scripts".

**Table A1.** Predictions obtained using ML/6-12.

Nr	Strain11	Stress11	StressPred
1	5e-14	6.0014e-09	41.894
2	0.0005	60.014	53.935
3	0.000 853 01	102.38	60.448
4	0.002 353	175.29	168.04
5	0.003 853	225.68	190.92
6	0.005 353	256.33	271.62
7	0.006 853	273.07	275.44
8	0.008 353	281.68	283.34
9	0.009 853	286.1	284.16
10	0.011 353	288.5	287.12
:	:	:	:
128	0.084 93	288.49	287.24
129	0.086 43	289.91	289.4
130	0.087 93	291.32	290.66
131	0.089 43	292.73	291.98
132	0.090 93	294.14	295.29
133	0.092 43	295.56	296.73
134	0.093 93	296.97	297.55
135	0.095 43	298.38	299.57
136	0.096 93	299.79	299.04
137	0.098 43	301.21	300.23
138	0.099 93	302.62	303.32

## Appendix B

Model 7 is an optimizable GPR with the following hyperparameters:

- Basis Function: Constant;
- Kernel Function: Non-Isotropic Matern 3/2;
- Kernel Scale: 0.003 356 1;
- Sigma: 522.5964;
- Standardize Data: Yes.

**Table A2.** The last two columns of the test dataset and the predicted values generated by model 7.

Nr	Strain11	Stress11	StressPred
1	0	0	-0.728 49
2	0.0005	60.014	61.518
3	0.000 853	102.38	101.05
4	0.002 353	175.29	175.53
5	0.003 853	225.68	225.67
6	0.005 353	256.33	254.81
7	0.006 853	273.07	273.44
8	0.008 353	281.68	280.06
:	:	:	:
69	0.099 853	330.95	331.33
70	0	0	0.4573
71	0.0005	30.21	29.859
72	0.001	60.42	61.265
73	0.002 430 1	133.88	133.33
74	0.003 930 1	174.71	173.34
:	:	:	:
134	0.093 93	296.97	297.51
135	0.095 43	298.38	298.95
136	0.096 93	299.79	299.86
137	0.098 43	301.21	301.11
138	0.099 93	302.62	302
139	0	0	0.392 46
140	5e-14	5.3419e-09	-0.160 96
141	0.0005	53.419	52.746

## Appendix C

The optimizable GPR has the following hyperparameters:

- Basis Function: Constant;
- Kernel Function: ARD Matern 3/2;
- Sigma: 0.668;
- Standardize Data: Yes.

**Table A3.** Predictions made by mdlGPR28 for data points related to CF/11 that are not part of the training set.

Nr	Strain11	Stress11	Prediction
1	5e-14	5.3419e-09	-0.155 13
2	0.0005	53.419	53.591
3	0.002 186 3	204.59	204.53
4	0.003 686 3	255.01	255.21
5	0.006 686 3	283.88	284.15
6	0.008 186 3	286.8	286.79
7	0.011 186	290.03	290.36
8	0.012 686	291.42	291.44
9	0.015 686	294.16	293.94
10	0.017 186	295.53	295.55
11	0.020 186	298.25	298.41
12	0.021 686	299.62	299.66
13	0.024 686	302.34	302.63
14	0.026 186	303.7	303.68
15	0.029 186	306.42	306.13
16	0.030 686	307.79	307.74
17	0.033 686	310.51	310.55
18	0.035 186	311.87	311.86
19	0.038 186	314.59	314.28
20	0.039 686	315.96	315.97
21	0.042 686	318.68	318.34
22	0.044 186	320.04	320.02
23	0.047 186	322.76	322.93
24	0.048 686	324.12	324.12
25	0.051 686	326.85	327.14
26	0.053 186	328.21	328.27
27	0.056 186	330.93	331.19
28	0.057 686	332.29	332.29
29	0.060 686	335.02	335.41

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**Continued**

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30	0.062 186	336.38	336.37
31	0.065 186	339.1	339.11
32	0.066 686	340.46	340.4
33	0.069 686	343.19	343.01
34	0.071 186	344.55	344.52
35	0.074 186	347.27	347.21
36	0.075 686	348.63	348.63
37	0.078 686	351.35	351.29
38	0.080 186	352.72	352.78
39	0.083 186	355.44	355.29
40	0.084 686	356.8	356.83
41	0.087 686	359.52	359.25
42	0.089 186	360.88	360.87
43	0.092 186	363.61	363.39
44	0.093 686	364.97	364.96
45	0.096 686	367.69	367.39
46	0.098 186	369.05	369.07

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