Prediction of mechanical properties of rail pads under in-service
 conditions through machine learning algorithms

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13 Highlights

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- This study focuses on rail pads fabricated in EPDM, TPE and EVA
 - Pads' stiffness was predicted through Machine Learning from the working conditions
- 16 The importance of each in-service condition was ascertained
- The dependency of each working condition on the stiffness was estimated.
- An application capable of predicting rail pad stiffness was developed

19 Abstract

20 Train operations generate high impact and fatigue loads that degrade the rail infrastructure and 21 the vehicle components. Rail pads are installed between the rails and the sleepers in order to 22 damp the transmission of vibrations and noise and to provide flexibility to the track. These 23 components play a crucial role in maximizing the durability of the railway assets and minimizing 24 maintenance costs. Rail pads can be fabricated with different polymeric materials that exhibit 25 non-linear mechanical behaviours, which strongly depend on the service conditions. Therefore, 26 it is extremely difficult to estimate their mechanical properties, in particular the dynamic 27 stiffness. In this work, several machine learning methodologies (multilinear regression, K nearest 28 neighbours, regression tree, random forest, gradient boosting, multi-layer perceptron and 29 support vector machine) were used to determine the dynamic stiffness of rail pads depending 30 on their in-service conditions (temperature, frequency, axle load and toe load). 720 31 experimental tests, under different realistic operating conditions, were performed to produce a 32 dataset that was then used for the training and testing of the machine learning methods. The 33 optimal algorithm was gradient boosting for EPDM (R² of 0.995 and mean absolute percentage 34 error of 5.08% in the test dataset), TPE (0.994 and 2.32%) and EVA (0.968 and 4.91%) pads. This 35 model was implemented in an application, available for the readers of this journal, developed 36 on the Microsoft .Net platform that allows the dynamic stiffness of the pads study to be 37 estimated as a function of the temperature, frequency, axle load and toe load.

Keywords: Railway dynamics; Sleeper pads; Machine learning; Rail service conditions; Dynamic
 stiffness.

40 1. Introduction

41 Given present trends, global demand for transport will more than double by 2050. The transport 42 sector is currently responsible for around one quarter of the global CO₂ emissions and such 43 growth will result in greater emissions unless profound changes are made in transportation 44 systems to achieve energy transitions globally. Rail is considered as one of the most energy 45 efficient modes of transport for freight and passengers and, as a consequence, it provides a 46 means to reduce the energy use and the environmental impact associated with transport. 47 According to the International Energy Agency [1], the rail sector carries 8% of the world's 48 passengers and 7% of global freight, but it represents only 2% of total transport energy demand.

49 The reduction of operation and maintenance (O&M) costs and the minimization of incidents, 50 which cause service delays and traffic disruption, brings very important challenges for rail 51 transport in order to address modern society demands and to increase its attractiveness and 52 competitiveness with respect to other means of transportation. A number of studies have been 53 developed to understand the influence of train operations on the response of the infrastructure 54 [2–10]. Other authors have devoted their attention to the detailed representation of the vehicle-55 track interaction using co-simulation methodologies encompassing multibody and finite 56 element formulations [11]. These developments enable the integration of more detailed wheel-57 rail contact models [12–21], to consider track irregularities [22,23] and other track singularities 58 [24–27] in the studies aiming to assess track performance and degradation evolution [28–31] 59 under realistic operation conditions. All these studies contribute to the development of novel 60 technology and to the reduction of O&M costs.

61 Rail pads are the elements with the greatest influence on the track stiffness, which is a 62 fundamental parameter for the maintenance of the track [32–38], in particular in the case of 63 ballastless track [39,40]. One of the main difficulties encountered when developing a reliable 64 numerical model of the mechanical response of the rail track is that the stiffness of the pads is 65 highly influenced by the operating conditions. Although the specific influence is strongly 66 material-dependent, some common trends have been experimentally described in the 67 literature: stiffness increases with frequency [41-43], axle load [44] or toe load [42], and 68 decreases with temperature [43]. Frequency can be as high as 80 kHz [45], but frequencies 69 above 20 Hz are considered as the result of track imperfections associated with small load 70 amplitude values. Even though rail pads have a fundamental role in the attenuation of this type 71 of frequencies, this work focuses on frequencies below 20 Hz, since this range is representative 72 of railway transportation and are associated with the highest load amplitudes. Testing at 73 extreme temperatures can seriously modify the response of the component, but since the 74 railway superstructure works at environmental temperatures, the characterization has been 75 conducted in the range between -35 and 52 °C.

Obtaining a reliable numerical prediction of the dynamic stiffness is an unresolved issue, not only because of the highly non-linear behaviour of these polymeric materials but also because of the interactions existing between the aforementioned variables [41,42,44,46–48]. Machine Learning (ML) methods are particularly well-suited for nonlinear and highly interactive data modelling. ML algorithms build a mathematical model based on a training dataset to make predictions on fresh data (testing dataset) without being explicitly programmed to perform the task.

In this study, a number of ML algorithms are developed to predict the dynamic stiffness of three
 types of commercial rail pads, EPDM, TPE and EVA, as a function of the in-service conditions,

85 namely frequency, axle load, temperature and toe load. The dataset comprised 720 86 experimental tests. The following seven algorithms were implemented for each material [49]: 87 Multi-Linear Regression (MLR), K Nearest Neighbours (KNN), Regression Tree (RT), Random 88 Forest (RF), Gradient Boosting (GB), Multi-Layer Perceptron (MLP) [50] and Support Vector 89 Machine (SVM) [51,52]. 80% of the observations are randomly chosen to form the training 90 dataset. The algorithms are optimised through three-fold cross-validation. The test dataset (20% 91 of the cases) was used to obtain an unbiased estimation of the predictive ability of the 92 algorithms. Specific ML methods are implemented to sort, for each of the three types of pads, 93 the operating conditions based on their relevance and to determine the specific influence of 94 each variable on the dynamic stiffness.

95 The reliable ML algorithms proposed here can be used for a large number of applications. First, 96 they can be a valuable tool for the definition of the type of rail pad to use, depending on the 97 operating conditions. In addition, they can be very useful for the evaluation of the track 98 conditions, increasing durability and providing information for maintenance management 99 procedures. In this sense, these tools can be easily linked to finite element models of the 100 infrastructure [53] in order to obtain the stress state on the track components depending on; 101 the loads generated by the train service, the environmental conditions and the assembly 102 settings. In this study, once the ML model with the best predictive ability had been obtained, an 103 application to estimate the dynamic stiffness of the EPDM, TPE and EV pads characterized as a 104 function of the operation conditions (frequency, axle load, temperature and toe load) was 105 developed. This app is freely available for readers.

The remainder of the paper is organized as follows. The materials and experimental techniques are described in section 2. The ML methods, the regression algorithms and the techniques implemented to identify the most relevant features as well as their influence on the dynamic stiffness are detailed in section 3. Section 4 is devoted to presenting the results of the analysis, their interpretation and the characteristics of the app. Finally, the conclusions of the research are summarized in section 5.

112 2. Materials and Experimental Tests

113 2.1. Materials

In this study, three of the most commonly used materials for rail pads were selected, namely;EPDM, TPD and EVA, see Figure 1.

- a) EPDM: ethylene-propylene copolymer, solid rail pad of 7 mm thickness without protrusions,
 with a hardness of 21 HS-D. This rail pad is used, for example, in Saudi Arabia's high-speed
 railways.
- b) TPE: Polyester elastomer thermopolymer (Hytrel[™]), with oblong shaped protrusions, a
 thickness of 7 mm, medium stiffness and a hardness of 47 HS-D. This is adopted, e.g., in the
 Spanish high-speed railways.
- c) EVA: Ethylene-vinyl acetate, solid rail pad of 6 mm thickness without protrusions and a
 hardness of 46 HSD. This rail pad forms part of the solution adopted, for example, in the first
 Spanish high-speed line between Madrid and Sevilla.



(a) (b) (c) Figure 1. Rail pads studied: (a) EPDM, 7 mm thick; (b) TPD, 7 mm thick; (c) EVA, 6 mm thick

126 2.2. Experimental Campaign

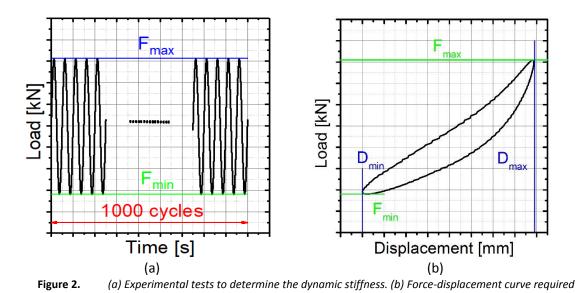
127 The procedures defined in standards EN 13481-2 [54] and EN 13146-9 [55] are used here to 128 obtain experimentally the dynamic stiffness (k_{dyn}) of the rail pads under different service 129 conditions. The procedure is schematically depicted in Figure 2(a) where 1000 sinus-type cycles 130 are applied between F_{min} and F_{max} . Then, 10 cycles belonging to the last 100 cycles are selected 131 and the average values of forces and displacements ($\overline{F_{max}}$, $\overline{F_{min}}$, $\overline{D_{max}}$, $\overline{D_{min}}$) are obtained as 132 shown in Figure 2(b). Finally, the following equation is applied to obtain the dynamic stiffness:

$$k_{dyn} = \frac{\overline{F_{max}} - \overline{F_{min}}}{\overline{D_{max}} - \overline{D_{min}}}$$
(1)

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134 To simulate different assembly and operating conditions of the pads, the values of frequency, 135 load amplitude, temperature and toe load are varied, as shown in Table 1. Fmin in Figure 2(a) 136 corresponds to the toe load and F_{max} is obtained by using the values of force amplitude defined 137 in EN 13481-2 [54], namely 15.5, 21 and 31.5 kN. This standard also proposes three values for 138 the frequency; 5, 10 and 20 Hz. In this study, a frequency of 2.5 Hz is also considered, as 139 suggested by previous studies [5,56]. The Spanish standard for the definition of action on bridges 140 considers as the minimum and maximum temperatures -35°C and 52°C, respectively, and the 141 EN 13481-2 [54] defines the dynamic stiffness test temperature as 23 ± 5 °C; to obtain regular 142 intervals between temperatures, -35 °C, -20 °C, 0°C, 20°C and 52 °C are considered in this 143 research. To obtain regular intervals between temperatures, 0°C and -20°C are also considered. 144 Four values for the toe load are also analyzed here. These correspond to the reference value (18 145 kN), representing a correct assembly of the fastening system, scenarios corresponding to the 146 fracture of the system (1 kN), an under-tightening (9 kN) or an over-tightening (25 kN). Since the 147 experimental campaign on the three pads is carried out for four frequencies, three load 148 amplitudes, five temperatures and four toe loads, it produces 3x4x3x5x4=720 test results. To 149 the best of the authors' knowledge, this is the most extensive and ambitious experimental 150 research conducted in this field.





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Experimental parameters with influence on the mechanical response of the rail pads Table 1.

to obtain the dynamic stiffness

| Frequency [Hz] | Amplitude [kN] | Temperature [ºC] | Toe load [kN] |
|----------------|----------------|------------------|---------------|
| 2.5 | 15.5 | -35 | 1 |
| 5 | 21.0 | -20 | 9 |
| 10 | 31.5 | 0 | 18 |
| 20 | | 20 | 25 |
| | | 52 | |

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Machine Learning Methods 3. 156

157 3.1. Machine Learning Algorithms

158 The ML algorithms are developed and evaluated in Python [57] using the libraries Numpy [58], 159 Pandas [59], Scikit-learn [60], Matplotlib [61] and Seaborn [62]. The dataset consists of 720 160 instances and five features: material, frequency, load amplitude, toe load and temperature. The 161 first variable, material, is categorical, i.e., it contains labels ('EPDM', 'TPE', 'EVA') rather than 162 numeric values. Many ML methods cannot operate on categorical data but require all variables 163 to be numeric. For this reason, the feature 'material' is one-hot encoded before any calculation.

164 Before processing, the five features are standardized to make them have zero-mean and unit-165 variance (StandardScaler). This technique is generally recommended and mandatory when 166 employing some specific algorithms [63]. The following regression algorithms have been 167 implemented in this research: Multiple Linear Regression (MLR), K-Nearest Neighbors (KNN), 168 Regression Tree (RT), Random Forest (RF), Gradient Boosting (GB), Support Vector Machine 169 (SVM), and Artificial Neural Networks (ANNs, in this case, Multi-Layer Perceptron, MLP). In the 170 following, a brief description of these algorithms is presented:

171 MLR is considered as a baseline algorithm for regression, i.e., a simple model which has a • reasonable chance of providing decent results. In MLR, the relationship between the 172 173 predictors (features) and the target / response variable is modeled through a linear equation 174 which is fitted to the observed data. The linear nature of MLR restricts its ability to describe 175 complex data.

In KNN, classification or regression are conducted for a new observation by summarizing the output variable of the 'K' closest observations (the neighbors) with uniform weights or with weights proportional to the inverse of the distance from the query point. Classification is carried out using the mode of the neighbors while regression is usually based on the mean.
 The distance between instances is expressed through the Minkowski metric which depends on the power parameter, 'p'. When p = 1, this is equivalent to using the Manhattan distance and for p=2 the Euclidean distance.

- A decision tree is a flowchart-like structure in which each node splits a feature in two branches until a leaf node is reached which represents a class label or a numeric value, depending on whether a classification or regression is being conducted. In RTs, the cost function that is minimized to choose split points is the sum squared error of the samples in the training dataset. The most important advantage of RTs is that they are easy to understand and to interpret. The drawback is that they easily tend toward overfitting. To avoid overfitting, several pruning techniques are available.
- 190 SVM was originally designed as a classifier [64] but may also be used for regression and • feature selection [65]. In classification, SVM determines the optimal separating hyperplane 191 192 between linearly separable classes maximizing the margin, which is defined as the distance 193 between the hyperplane and the closest points on both sides (the support vectors). For non-194 perfectly separable classes, SVM must be modified to allow some points to be misclassified, 195 which is achieved by introducing a "soft margin" [66]. Datasets that are highly nonlinear may 196 in some cases be (linearly) separated after being (nonlinearly) mapped into a higher 197 dimensional space [67]. This mapping gives rise to the kernel, which can be chosen by the 198 user among different options such as linear, sigmoid, Gaussian or polynomial. The 199 appropriate kernel function is selected by trial and error on the test set. In this case, SVM is 200 referred to as kernelized SVM.
- 201 Ensemble methods combine multiple "weak classifiers" into a single "strong classifier". A 202 weak classifier is a classifier that performs poorly, but performs better than random 203 guessing. Ensemble methods are classified into bagging-based and boosting-based, which 204 are designed to reduce variance and bias, respectively. Bagging stands for Bootstrap 205 Aggregating. RF is a widely used bagging method based on classification trees (weak 206 learner). In RFs, each tree in the ensemble is built from a bootstrap sample of the training 207 set. In addition, instead of using all the features, a random subset of features is selected, 208 further randomizing the tree. In boosting, each new tree is a fit on a modified version of the 209 original data set. Gradient Boosting trains many models in a sequential manner identifying 210 the shortcomings of weak learners using gradients in the loss function.
- 211 ANNs are mostly used for data classification and pattern recognition [68]. A basic ANN • 212 contains a large number of neurons / nodes arranged in layers. MLP contains one or more 213 hidden layers (apart from one input and one output layer). The nodes of consecutive layers 214 are connected and these connections have weights associated with them. In a feedforward 215 network, the information moves in one direction from the input nodes, through the hidden 216 nodes (if any) to the output nodes. The output of every neuron is obtained by applying an 217 activation function to the linear combination of inputs (weights) to the neuron. Sigmoid, 218 tanh and ReLu (Rectified Linear Unit) are the most widely used activation functions. MLPs 219 are trained through the backpropagation algorithm. Gradient descent, Newton, conjugate 220 gradient and Levenberg-Marquardt are different algorithms used to train an ANN.
- 20% of the observations are randomly extracted to form a test dataset that was used to providean unbiased evaluation of the models. Models are trained and the hyper-parameters are refined

using the remaining 80% of the data. 3-fold cross-validation (CV3) was used for training and
validation to guarantee the ability of the algorithm to generalize and to avoid overfitting.
Parameter selection and model evaluation was conducted with GridSearchCV [69].

226 3.2. Feature Importance and Permutation Importance

227 The assessment of feature relevance provides insight into which factors most influence the 228 output [70]. Feature Importance (FI) and Permutation Importance (PI) are two independent 229 methods which only require an estimator that has been satisfactorily fitted. Both techniques are 230 implemented in Scikit-Learn. Tree-based models, such as RF and GB, provide the FI score, which 231 is based on the mean decrease in impurity after a split. The PI of a feature is measured as the 232 decrease in the model score when a single feature value is randomly shuffled. Thus, the larger 233 the drop is in the score, the higher is the relevance of the feature. The amount of randomness 234 in FI or PI is calculated by repeating the process at random several times.

235 3.3. Partial Dependence Plots

236 A one-way Partial Dependence Plot (PDP) is a graph that displays the relationship between one 237 feature and the target response. The x-axis represents the values of the feature, while the y-axis 238 displays the partial dependence. PDPs are calculated using a model that has been previously 239 fitted. For each value of the target feature, the PDP is obtained after marginalizing the 240 predictions of the fitted model over the actual values of the rest of the features. Then, a 241 distribution of values is obtained (one value for each of the instances of the dataset). This 242 operation is repeated at intervals of values in the range of the target feature. Scikit-Learn 243 provides a specific function to create a PDP.

244 4. Results and Discussion

245 4.1. Selection of the Optimal Model for each Material

The coefficient of determination, R^2 , is selected as the regression score function for the optimization of the hyperparameters of the algorithms. These hyperparameters are listed in Table 2.

Table 2.Hyperparameters obtained after optimizing each ML algorithm for each pad

| MLR | N/A. | | | |
|-----|---|--|--|--|
| KNN | EPDM: 'metric': 'manhattan', 'n_neighbors': 2, 'weights': 'uniform'. TPE: 'metric': 'manhattan', 'n_neighbors': 2, 'weights': 'uniform'. EVA: 'metric': 'manhattan', 'n_neighbors': 4, 'weights': 'distance'. | | | |
| RT | EPDM: 'criterion': 'mse', 'max_depth': 10, 'min_samples_leaf': 2, 'min_samples_split': 5, 'splitter': 'best'. TPE: 'metric': 'manhattan', 'n_neighbors': 2, 'weights': 'uniform'. EVA: 'criterion': 'mse', 'max_depth': 10, 'min_samples_leaf': 2, 'min_samples_split': 5, 'splitter': 'best'. | | | |
| RF | EPDM: 'bootstrap': False, 'max_depth': 15, 'max_features': 3, 'min_samples_split': 2, 'n_estimators': 5. TPE: 'bootstrap': True, 'max_depth': 10, 'max_features': 3, 'min_samples_split': 2, 'n_estimators': 50. EVA: 'bootstrap': True, 'max_depth': 15, 'max_features': 3, 'min_samples_split': 2, 'n_estimators': 10. | | | |
| GB | EPDM: 'learning_rate': 0.5, 'max_depth': 6, 'max_features': 3, 'min_samples_leaf': 5, 'min_samples_split': 2, 'n_estimators': 100. | | | |

| | TPE: 'learning_rate': 0.1, 'max_depth': 10, 'max_features': 3, 'min_samples_leaf': 5, 'min_samples_split': 10, 'n_estimators': 500. | | | | |
|-----|--|--|--|--|--|
| | EVA: 'learning_rate': 0.5, 'max_depth': 2, 'max_features': 3, 'min_samples_leaf': 10, 'min_samples_split': 3, 'n_estimators': 500. | | | | |
| | | | | | |
| MLP | EPDM: 'activation': 'relu', 'alpha': 0.005, 'hidden_layer_sizes': (10, 10, 10), | | | | |
| | 'max_iter': 50000, 'solver': 'lbfgs'. | | | | |
| | TPE: activation='relu', alpha=0.005, hidden_layer_sizes=(10, 10), | | | | |
| | max_iter=100000, solver='lbfgs'. | | | | |
| | EVA: 'activation': 'relu', 'alpha': 0.0001, 'hidden_layer_sizes': (10, 10), | | | | |
| | 'max_iter': 25000, 'solver': 'adam'. | | | | |
| SVM | EPDM: 'degree': 2, 'gamma': 'auto', 'kernel': 'linear'. | | | | |
| | TPE: 'degree': 2, 'gamma': 'auto', 'kernel': 'linear'. | | | | |
| | EVA: 'degree': 2, 'gamma': 'auto', 'kernel': 'linear'. | | | | |

After optimization, the coefficient of determination (R²), Root Mean Square Error (RMSE), Mean Absolute Error (MAE) and Mean Absolute Percentage Error (MAPE) are calculated in the test dataset. This information is shown in Table 3, Table 4 and Table 5 for EPDM, TPE and EVA pads, respectively. As can be seen, GB stands out above the rest of the algorithms for all three materials. For EPDM and TPE, R² is 0.995 while for EVA it is 0.988. Also note that, for the selected algorithms, the MAPE is between 2.3% and 6.5%.

Table 3.Statistical scores in the test dataset provided by each model for the EPDM pad

| Algorithm | R ² | RMSE [kN/mm] | MAE [kN/mm] | MAPE [%] |
|-----------|----------------|--------------|-------------|----------|
| MLR | 0.452 | 100.39 | 133.67 | 88.78 |
| KNN | 0.628 | 61.58 | 110.14 | 34.76 |
| RT | 0.923 | 22.75 | 50.07 | 9.24 |
| RF | 0.965 | 16.45 | 33.66 | 6.18 |
| GB | 0.995 | 12.36 | 7.39 | 5.08 |
| MLP | 0.990 | 10.23 | 17.96 | 6.51 |
| SVM | 0.060 | 81.28 | 175.13 | 30.44 |

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Table 4.Statistical scores in the test dataset provided by each model for the TPE pad

| Algorithm | R ² | RMSE [kN/mm] | MAE [kN/mm] | MAPE [%] |
|-----------|----------------|--------------|-------------|----------|
| MLR | 0.759 | 40.18 | 52.02 | 17.83 |
| KNN | 0.872 | 27.73 | 37.99 | 10.18 |
| RT | 0.969 | 12.48 | 18.52 | 4.72 |
| RF | 0.977 | 9.86 | 16.18 | 3.45 |
| GB | 0.995 | 7.79 | 5.41 | 2.25 |
| MLP | 0.994 | 5.8 | 8.02 | 2.32 |
| SVM | 0.545 | 42.2 | 71.49 | 13.99 |

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Table 5.Statistical scores in the test dataset provided by each model for the EVA pad

| Algorithm | R ² | RMSE [kN/mm] | MAE [kN/mm] | MAPE [%] |
|-----------|----------------|--------------|-------------|----------|
| MLR | 0.928 | 76.62 | 93.24 | 7.88 |
| KNN | 0.927 | 67.93 | 93.64 | 7.04 |
| RT | 0.922 | 75.15 | 97.02 | 7.17 |
| RF | 0.968 | 50.23 | 62.52 | 4.91 |
| | | | | |

| GB | 0.988 | 37.36 | 20.37 | 2.38 |
|-----|-------|--------|--------|-------|
| MLP | 0.927 | 78.3 | 93.72 | 7.97 |
| SVM | 0.56 | 188.92 | 230.44 | 22.85 |

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Figure 3, Figure 4 and Figure 5 illustrate the prediction ability of the different ML algorithms for EPDM, TPE and EVA pads, respectively. The experimental values of stiffness are represented on the X-axis and the predictions of each of the regressors are shown on the Y-axis. Each graph

266 includes a 1:1 line (corresponding to a perfect fitting) as well as two confidence bands separated

from the centre line by a distance equal to the RMSE defined in Table 3, Table 4 and Table 5.

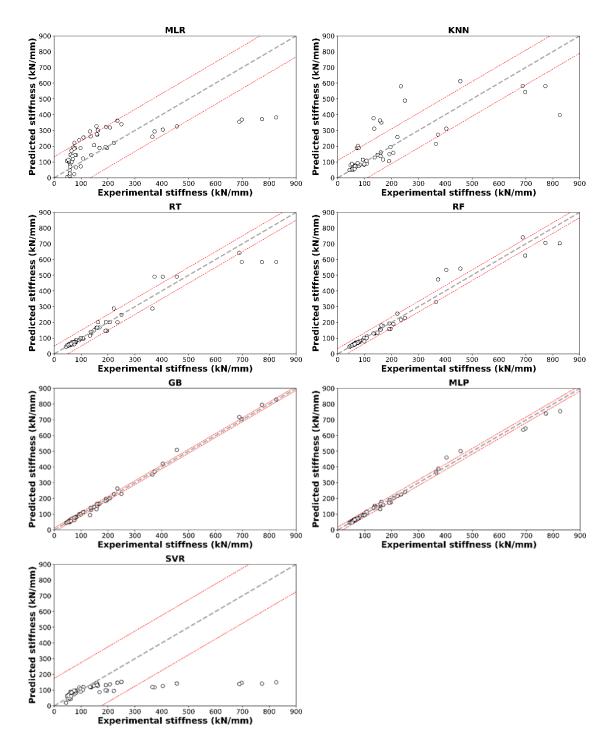
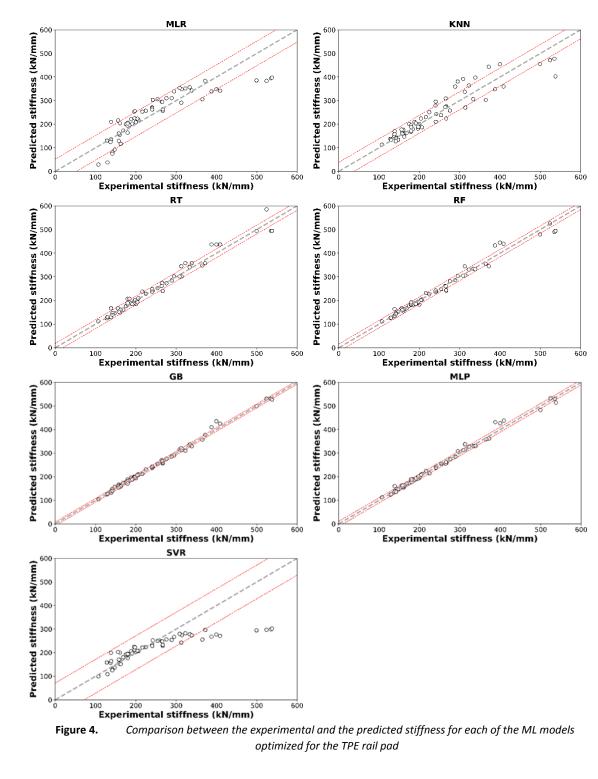
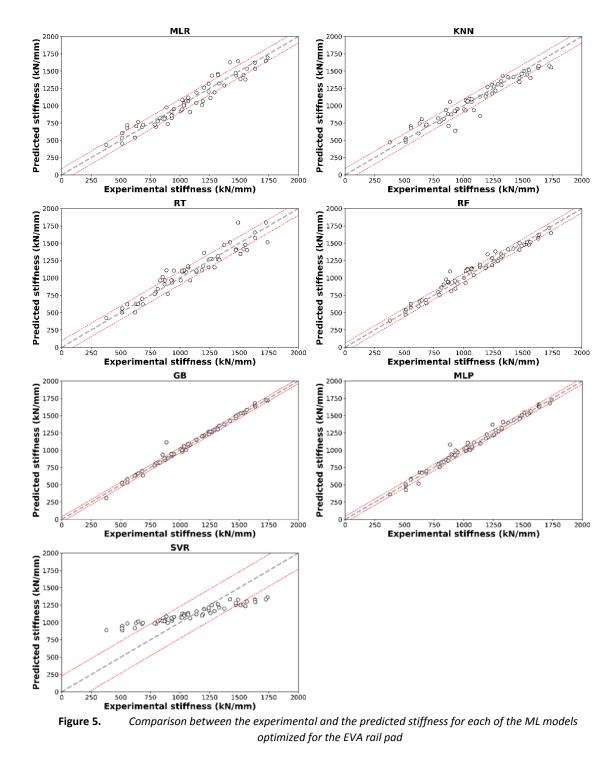


Figure 3.

Comparison between the experimental and the predicted stiffness for each of the ML models optimized for the EPDM rail pad







278 4.2. Partial Dependence Plots

It is generally known how service variables (temperature, toe load, frequency and axle load) influence the dynamic stiffness of the rail pads. For higher axle loads, the stiffness is higher. This phenomenon is explained because, for high loads, the capacity of the rail pads to deform is lower and, therefore, the rail pads have a more rigid response. On the other hand, the higher the frequency, the greater the stiffness obtained. This is explained because, if the load frequency is high, the pads have less time to adapt to the movement and, therefore, less displacements are obtained. Regarding temperature, the higher it is, the greater is the capacity to deform and,

therefore, the lower is the stiffness. Finally, in a similar way to what happens with the axle load,

by increasing the toe load, the capacity of the pad to deform reduces and more rigid behaviouris observed.

As mentioned before, PDPs enable answers to be obtained about how and how much the influence of each of the variables is. Figure 6, Figure 7 and Figure 8 show the PDPs of the features for the three pads. In each of the graphs, a central trend thick line is represented, which is accompanied by a number of thin lines that provide a measure of the dispersion to the central line. The dark blue line is the average value of all generated cases, while the light blue ones are random cases

From Figure 6 it is observed that the evolution of the EPDM pad stiffness with both amplitude and frequency are approximately proportional. In case of temperature, it can be seen that for very low temperatures there is a significant variation. Once -20°C is exceeded, the effect of temperature is significantly reduced. Regarding the toe load effect, it is shown that there are two clearly differentiated phases. A first one up to approximately 12 kN and another one from that value, where the influence of that toe load is accentuated.



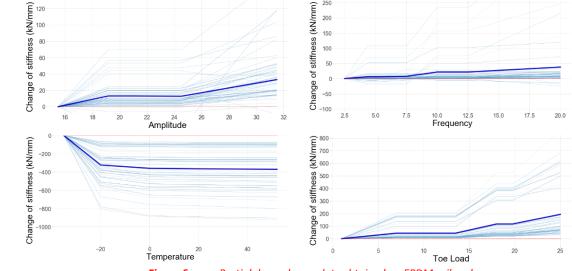
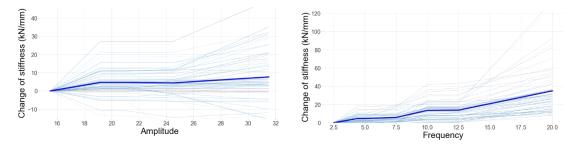
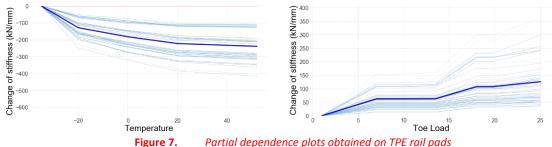




Figure 6. Partial dependence plots obtained on EPDM rail pads

Figure 7 shows that the effect on TPE pads of the increase in axle load, frequency and toe load
is approximately proportional. In contrast, it can be seen that the influence of temperature is
greater when the temperature is lower.

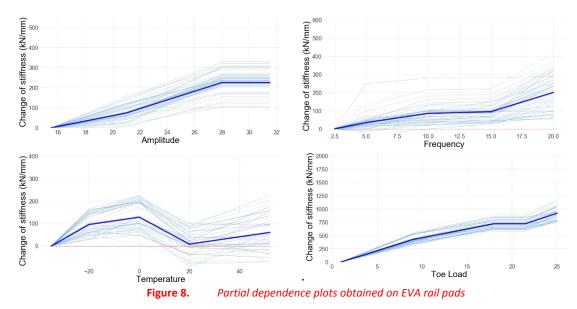






Partial dependence plots obtained on TPE rail pads

307 From Figure 8 it can be seen that the influence of amplitude, frequency and toe load on the EVA 308 pad is approximately proportional within the range studied. It can be seen that the PDP 309 corresponding to temperature does not seem to match with what could be expected, this is 310 because the influence of temperature is so small that it is screened by the uncertainty of the 311 measurement.



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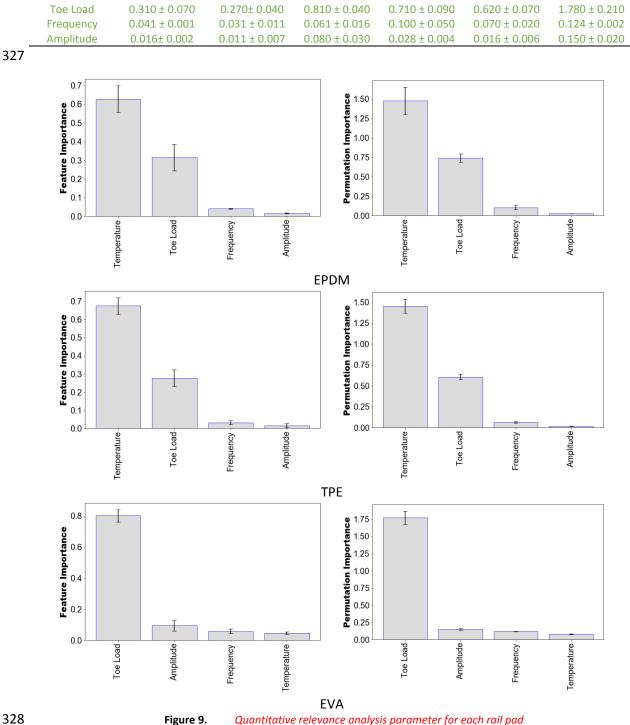
314 4.3. Feature and Permutation Importance

315 The results obtained with FI and PI are summarized in Table 6 and represented as bar charts in 316 Figure 9. Both algorithms display consistent results which is evidence of reliability, provided that 317 the fundamentals on which FI and PI are grounded are different and independent.

318 From the analysis of Figure 9, it is possible to determine which variables (temperature, toe load, 319 frequency and axle load) have most influence on the pads' dynamic stiffness. For the EPDM pad, 320 these parameters are temperature and toe load. Similarly, in the case of TPE, the parameters 321 that have most influence on the stiffness are temperature and toe load. In the case of the EVA 322 pad, the parameter with the greatest influence on the stiffness is temperature. It should be 323 noted that the most influential parameters on pad behaviour are temperature and toe load and 324 that the standard for characterizing these components only contemplates testing at different 325 temperatures in extreme cases and does not propose any variation of the toe load.

Table 6. Quantitative relevance analysis parameter for each rail pad

| | Feature Importance | | | Perm | utation Impor | tance |
|-------------|--------------------|---------------|---------------|-------------------|-------------------|---------------|
| | EPDM | TPE | EVA | EPDM | TPE | EVA |
| Temperature | 0.630 ± 0.070 | 0.690 ± 0.040 | 0.042 ± 0.009 | 1.430 ± 0.370 | 1.440 ± 0.190 | 0.088 ± 0.009 |



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4.4. Application for the implementation of the optimal ML algorithm

An application was created on the Microsoft .Net platform. The Visual Studio 2017 development environment was used with the C# programming language. The user interface is based on Windows Forms. The operating requirements are a 64-bit computer with .Net Framework 4.7 or higher (for example, any 64-bit Windows 10 computer meets this requirement). Click Once technology was used to deploy and download this application via Web. This mechanism enables the app to be updated. The predictive machine learning model has been created using the ML.Net library. It is an open source multiplatform library [71]. The algorithm employed was an efficient implementation of the Gradient Boosting algorithm called MART [72,73]. This
application can be downloaded from the following link: "http://www.cuartas.es/railpad/" in
Microsoft Edge.

341 5. Conclusions and Future Developments

At present, there are no models, neither analytical nor numerical, that enable the dynamic stiffness of rail pads to be obtained depending on the assembly and operation conditions. However, this would be helpful because the polymeric materials used to manufacture these pads display a highly non-linear mechanical response and interactions among the service variables occur. Previous studies have experimentally obtained the influence of one or another of these variables. But this experimental information, scarce and dispersed, has not enabled reliable models to be produced.

349 The experimental scope of the present work includes a total of 720 dynamic tests carried out on 350 three of the most common pad materials. The difficulties in modelling the response of these 351 materials using conventional procedures justify the adoption of alternative data-driven 352 methodologies. For this purpose, several machine learning algorithms are implemented and 353 optimized. Gradient Boosting was found to be the optimal algorithm for the three materials. In 354 general, Random Forest, which is also an ensemble method, and Multilayer Perceptron have 355 provided very notable results. The ability of Gradient Boosting is highlighted by the coefficient 356 of determination and mean absolute percentage error in the test dataset, which are 357 0.995/5.08%, 0.995/2.25% and 0.988/2.38%, for EPDM, TPE and EVA, respectively.

358 Two alternative methodologies, feature importance and permutation importance, which enable 359 the features to be sorted by order of importance, are also implemented. These procedures 360 provide consistent results. Temperature and toe load are the variables that most influence the 361 dynamic stiffness of EPDM and TPE, while toe load is the most relevant feature for EVA. Overall, 362 toe load is the most influential parameter, regardless of the material tested. This result is 363 particularly remarkable since the standards that define the experimental conditions for 364 determination of the dynamic stiffness of rail pads do not take it into account. In the authors' 365 opinion, the experimental and analytical evidence provided by this study is sufficient to motivate 366 a possible update of the standards currently in force.

This information is useful for track design and for providing information about the maintenance procedures to the infrastructure managers. In addition, the algorithms developed here can be easily coupled with finite element models that include all the track components. This would enable the determination of the overall impact of the variables considered here, temperature, axle load, toe load and frequency on the infrastructure behaviour. These developments would support the optimization of the maintenance tasks and contribute to increasing the durability of tracks.

374 Considering the potential interest of the results of this research for the railway industry, an 375 application implementing the optimal Machine Learning algorithm was developed. This 376 application enables the prediction of the dynamic stiffness of the rail pads covered in this study 377 (manufactured either in EPDM, TPE or EVA) from the operating conditions.

In this paper, a methodology combining laboratory testing with machine learning algorithms has
been implemented. This combination has provided a computational mechanical model for each
of the materials. This technique can be extended to model other mechanical properties
particularly difficult to be described in analytical terms. In this sense, this research is currently

being extended, modifying the values of frequency and load amplitude to analyse, not only thestiffness, but also the damping capacity of each kind of rail pad.

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