

1 Stacking ensemble with parsimonious base models  
2 to improve generalization capability in the  
3 characterization of steel bolted components

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8 **Abstract**

9 This study presents a new soft computing method to create an accurate  
10 and reliable model capable to determine three key points of the compre-  
11 hensive force-displacement curve of bolted components from steel struc-  
12 tures. To this end, a database with the results of a set of finite element  
13 (FE) simulations, which represent real responses of bolted components,  
14 is utilized to create a stacking ensemble model that combines the predic-  
15 tion of different parsimonious base models. The innovative proposal of  
16 this study is to use GA-PARSIMONY, a previously published GA-method  
17 which searches parsimonious models by optimizing feature selection and  
18 hyperparameter optimization processes. Therefore, parsimonious solu-  
19 tions created with a variety of machine learning methods are combined  
20 by means of a nested cross-validation scheme in a unique meta-learner in  
21 order to increase diversity and minimize the generalization error rate. The  
22 results reveal that efficiently combining parsimonious models provides  
23 more accurate and reliable predictions as compared to other methods.

24 Therefore, the informational model is able to replace costly FE simulations  
25 without significantly comprising accuracy, and could be implemented in  
26 structural analysis software.

27 *Keywords:*

28 Stacking ensemble model, Parsimonious models, Bolted connection,  
29 GA-PARSIMONY, T-stub

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## 30 **1. Introduction**

31 Structural steel connections play an essential role in the stability of  
32 frames and buildings. Since the introduction of the semi-rigid concept [1]  
33 numerous methods have been developed to accurately predict the moment-  
34 rotation response of steel connections [2]. The semi-rigid approach repre-  
35 sented an important breakthrough in the design of these elements which  
36 led to significant reductions in weight and costs. Nevertheless, complex  
37 and advanced analyses were required to tackle the nonlinearities involved  
38 in the calculation process.

39 Nowadays, the use of component-based models for the assessment  
40 of semi-rigid steel connections is widely accepted among practitioners.  
41 Their principle basis consists of dividing the connection into individual  
42 components represented as springs, each one characterized by their force-  
43 displacement response in terms of initial stiffness and maximum strength.  
44 The moment-rotation curve of the connection is then determined by as-  
45 sembling the individual responses of all components in a mechanical sys-  
46 tem. For example, in beam-to-column bolted joints (Fig. 1a), tensile com-  
47 ponents represent the main source of deformability; hence, they are re-

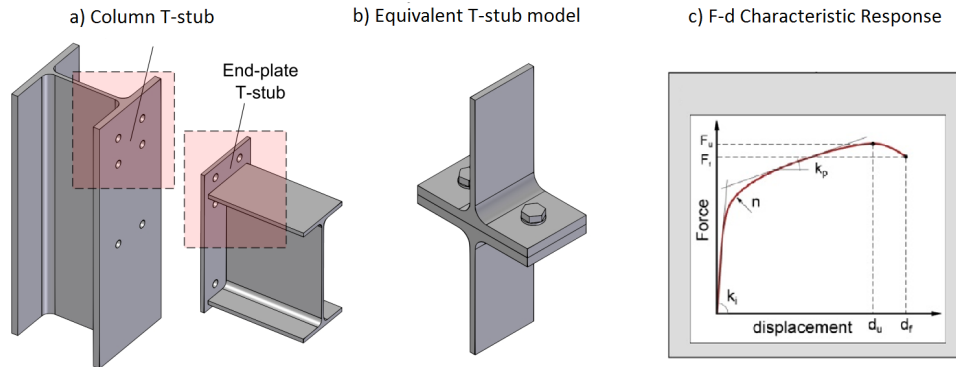


Figure 1: Tension zone in steel connections. (a) End-plate beam-to-column connection, (b) Equivalent T-stub model and (c) Force-displacement curve of the T-sub model to be obtained.

48 spondible for the rotation capacity of the entire joint. These components  
 49 can be effectively characterized by means of the equivalent T-stub model  
 50 (Fig. 1b).

51 Regulatory codes such as Eurocode 3 [3] have adopted this approach  
 52 which is suitable for hand calculation and reasonably accurate in deter-  
 53 mining rotational stiffness and moment resistance. However, further re-  
 54 search is still necessary to adequately characterize components and obtain  
 55 the connections comprehensive non-linear response, including its rotation  
 56 capacity (Fig. 1c). Alternatives to the existing analytical models [4] should  
 57 be able to handle material plasticity, contacts, progressive damage and fail-  
 58 ure. At the same time, practitioners need cost-effective methods in terms  
 59 of computational effort that are also suitable to be implemented into steel  
 60 structure software.

61 To date, numerical simulations based on the finite element (FE) method

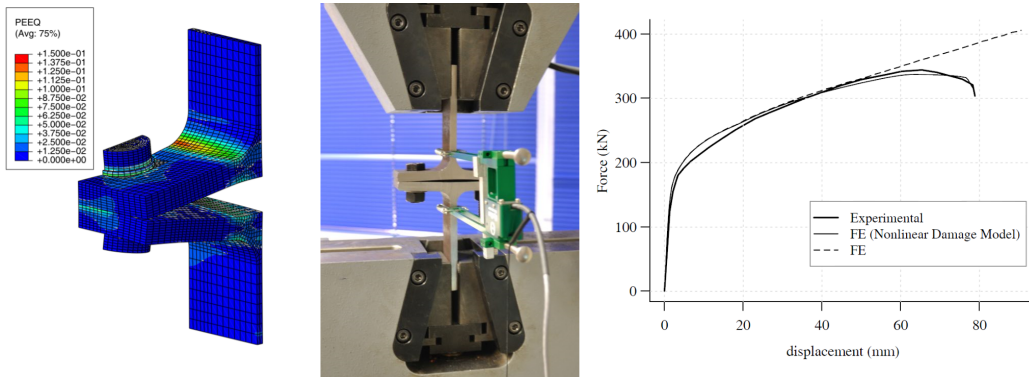


Figure 2: Characterization of the force-displacement curve of a bolted component with an FE model validated with experimental tests.

62 represent one of the most accurate ways to predict the behavior of steel  
 63 connections (Fig. 2). Nevertheless, the FE method continues to be a time-  
 64 consuming process in spite of growing computer power. The complexity  
 65 of the analysis codes seems to keep pace with continuous advances in soft-  
 66 ware and hardware [5]. Thus, the FE method remains inefficient in terms  
 67 of current requirements when design and optimization are required for  
 68 hundred of joints in a steel structure. Hence, a second level of abstrac-  
 69 tion is needed that would alleviate the computational burden required by  
 70 numerical simulations.

71 Machine learning models created from an FE simulation database rep-  
 72 resent a low-cost approximation of computationally expensive simulations  
 73 [6]. These models capture the underlying relationship between input vari-  
 74 ables and FE simulation results that can be expressed mathematically as:

$$y = f(x, \varphi) + \epsilon \quad (1)$$

75 where  $y$  is the actual value of the output,  $f$  contains the modeling function,

76  $x = [x_1, \dots, x_n]$  represents the array of  $n$  input variables,  $\Phi = [\varphi_1, \dots, \varphi_m]$   
77 denotes the array of  $m$  unknown parameters to adjust the function  $f$ , and  
78  $\epsilon$  includes both the error of fitting the machine learning model to the sim-  
79 ulation results and the intrinsic error corresponding to the simulation.

80 Concerning steel structures, artificial neural network (ANN) models  
81 were utilized by Shahin et al. [7] to predict the ultimate pure bending of  
82 steel circular tubes. A specific example of the design of semi-rigid joints  
83 can be found in the work reported by Diaz et al. [8] who employed krig-  
84 ing and genetic algorithms (GA) for cost-optimization of bolted end-plate  
85 connections. Recently, Fernandez-Ceniceros et al. [9, 10] have also offered  
86 insight into the use of machine learning models for the assessment of steel  
87 bolted connections.

88 Model generalization capability corresponds with the ability to pre-  
89 dict correct responses for new designs. This capability will depend on  
90 the machine learning algorithm, the model complexity and the training  
91 process. In the context of modeling the steel bolted connection behav-  
92 ior, the challenge is to obtain models capable of predicting highly accu-  
93 rate force-displacement curves for new designs trained with a relatively  
94 small database, which has been created with FE simulations. Selecting  
95 the most appropriate method for each case study remains a defiance for  
96 practical design. This model accuracy is generally influenced by several  
97 factors, such as the nature of the output variables, the number of com-  
98 putational FE experiments necessary to approximate the model, and the  
99 dimensionality of the problem in terms of number of input features. Re-  
100 garding the former, highly non-linear problems may require more flexible

101 modeling techniques to capture their complex behavior. However, flexible  
102 techniques provide excellent fit for computer experiments at the expense  
103 of lower generalization capacity. Therefore, a methodology to obtain an  
104 efficient trade-off between flexibility and generalization capability is in-  
105 evitable in order to overcome the phenomenon of over-fitting.

106 This article presents a new hybrid methodology which couples numer-  
107 ical and informational models to predict key parameters of steel connec-  
108 tions such as initial stiffness, maximum resistance and displacement at  
109 failure. To this end, numerical models based on the finite element method  
110 (FEM) are developed first to reproduce the real response of bolted com-  
111 ponents selected with a design of experiments. These models incorporate  
112 progressive damage mechanisms and failure criteria to accurately estimate  
113 the displacement at fracture. In order to minimize the computational bur-  
114 den of the FEM, the results of a set of simulations are utilized to create a  
115 database and then, construct a stacking ensemble model, also called meta-  
116 ensemble model, capable of determining the curve parameters with accu-  
117 racy for unseen data.

118 The primary innovation of this proposal is that it uses a soft comput-  
119 ing (SC) method previously published by the authors, GA-PARSIMONY  
120 [11], to obtain parsimonious and accurate base solutions with different  
121 algorithms, such as ANN, support vector machines (SVM), CUBIST, gra-  
122 dient boosting machines (GBM) and ridge regression, among others. GA-  
123 PARSIMONY obtains accurate parsimonious models for the first level by  
124 selecting the best features and parameters with a special parsimonious  
125 model selection (PMS) process based on a dual criteria which considers ac-

126 curacy and complexity separately. Finally, the predictions of the best par-  
127 simonious models obtained with each algorithm are combined with a sec-  
128 ond level stacking ensemble learner, also optimized with GA-PARSIMONY,  
129 in order to reduce variance and improve the generalization capability.

130 The rest of the article is organized as follows: Section 2 begins by  
131 introducing methods for improving model generalization capability and  
132 how its related with new SC techniques. Section 3 presents the proposed  
133 methodology which combines FE method to construct a database and, by  
134 using it with GA-PARSIMONY, to build an accurate stacking ensemble  
135 model based on parsimonious base models created with different machine  
136 learning algorithms. Section 4 describes the experiments performed for  
137 the case study of a T-stub component. Then, Section 5 deals with the  
138 results of the proposed method and compares them with previous ap-  
139 proaches. And lastly, Section 6 presents the conclusions and contributions  
140 of this research.

## 141 **2. Related research on using soft computing for improving generaliza-** 142 **tion capability**

143 In machine learning, the generalization capability is the ability of the  
144 model to handle unseen data. A model can perform well with the training  
145 data, but it may fail to predict the response in a new dataset. This capa-  
146 bility depends on a correct training process and on the model complexity.  
147 Thus, a poor generalization is obtained when the model is over-trained or  
148 when its degree of freedom is higher than that of the training data [12].  
149 This second aspect is related to the complexity of the model, which can

150 be defined by the internal structure [13] as the number of leafs or lev-  
 151 els in model trees or the sum of squared coefficients in ridge regression,  
 152 among others. For instance, the sum of squared weights is used in neu-  
 153 ral networks because too large weights can magnify the noise from the  
 154 inputs and propagate it to the output [14]. Therefore, this metric defines  
 155 the "flatness" of the model, which is directly related to the variance of the  
 156 prediction. Other complexity metrics are the *Vapnik-Chervonenkis* (VC) di-  
 157 mension [15], the *degrees of freedom* (GDF) [16] or the number of input fea-  
 158 tures selected ( $N_{SF}$ ), which is included in the penalty terms of the *Akaike*  
 159 *information criterion* [17] and the *Bayesian information criterion* (BIC) [18].

160 In this context, it is well known that, among several accurate models,  
 161 the least complex model (more parsimonious) should be selected. This  
 162 model will probably be more robust and reliable against new data, pertur-  
 163 bations and noise.

### 164 2.1. Trade-off between bias and variance

165 Models should be tested with unseen patterns in order to find their  
 166 generalization capability. Suppose that a real value  $y$  is explained as  $y =$   
 167  $f(\mathbf{x}) + \epsilon$ , where  $f(\mathbf{x})$  is the real function of the problem with  $n$  indepen-  
 168 dent attributes  $x_i$ , and  $\epsilon$  is the intrinsic error with zero mean and variance  
 169  $\sigma^2$ . Minimizing a metric such as the Mean Squared Error (MSE) allows to  
 170 search models  $\hat{f}(x)$  as close as possible to  $f(x)$ . Then, the expected MSE  
 171 with an unseen sample  $\mathbf{x}$ , also known as generalization error (GE), can be  
 172 decomposed as follows [19]:

$$E[(y - \hat{f}(\mathbf{x}))^2] = Bias[\hat{f}(\mathbf{x})]^2 + Var[\hat{f}(\mathbf{x})] + \sigma^2 \quad (2)$$



173 with:

$$Bias[\hat{f}(\mathbf{x})] = E[\hat{f}(\mathbf{x}) - f(x)] \quad (3)$$

174

$$Var[\hat{f}(\mathbf{x})] = E[\hat{f}(\mathbf{x})^2] - E[\hat{f}(\mathbf{x})]^2 \quad (4)$$

175 where the  $Bias^2$  is related to the accuracy of the model,  $Var$  is the vari-  
176 ance and represents the model repeatability or how much  $\hat{f}(x)$  will move  
177 around the mean, and  $\sigma^2$  is the irreducible error that was present in the  
178 original data.

179 The complexity of the model has opposite effects in the reduction of  
180 bias and variance. Figure 3 shows the training error and U-shaped MSE  
181 curves for two test samples of unseen data in relation with model complex-  
182 ity (horizontal axis). A high-flexible model like  $M_3$  obtains a low training  
183 MSE but the variance increases in the test samples. On the other hand,  
184 a low complex model as  $M_1$  shows a high bias because it cannot adapt  
185 correctly to the data. Controlling the the bias-variance trade-off is there-  
186 fore necessary to obtain strong overall models within the zone of lower  
187 generalization errors, as it occurs with model  $M_2$ . This control is called  
188 regularization and it takes into account both, complexity and accuracy of  
189 prediction, in the training process.

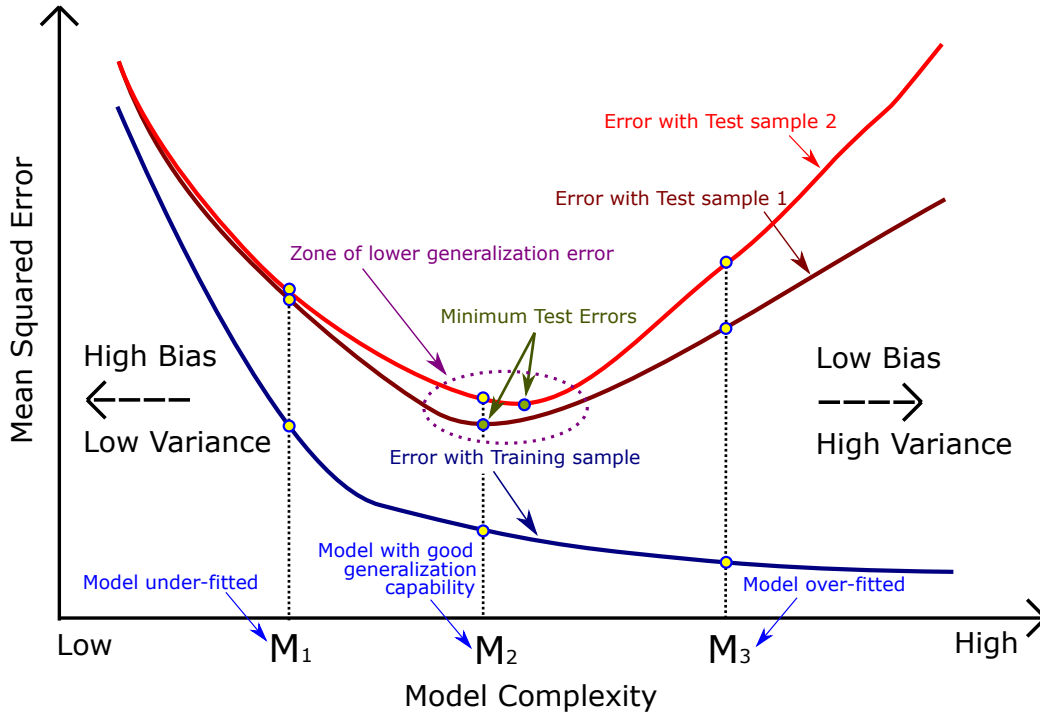


Figure 3: Bias-Variance and its relation with the model complexity.  $M_1$  is a under-fitted simple model with high bias but low variance.  $M_3$  is a over-fitted high-flexible model with low bias but high variance in unseen data.  $M_2$  obtains a trade-off between bias and variance to achieve good expected error with the test samples.

190 2.2. Regularization of wrapper models using soft computing

191 Regularization is included in the training process by minimizing a reg-  
 192 ularized "Loss+Penalty" function [19]:

$$\underset{\beta_0, \beta_1, \dots, \beta_p}{\text{minimize}} \{L(\mathbf{X}, \mathbf{y}, \beta) + \lambda P(\beta)\} \quad (5)$$

193 where  $\mathbf{X}$  is the input data,  $\mathbf{y}$  the response variable, and  $\beta$  the model weights.  
 194 The objective is to reduce  $L(\mathbf{X}, \mathbf{y}, \beta)$ , which is the loss function that quan-  
 195 tifies how the model fits the training data  $(\mathbf{X}, \mathbf{y})$ , and  $P(\beta)$ , which is the

196 penalty term for the complexity of the model.  $\lambda$  is a non-negative parame-  
197 ter that balances both terms and must be adjusted along with other tuning  
198 parameters.

199 An increasing number of studies have reported SC strategies where the  
200 optimization process considers the whole KDD-wrapper scheme. These  
201 schemes generally include not only hyperparameter optimization (HO)  
202 but also other tasks such as feature selection (FS), feature engineering (FE),  
203 data transformation (DT), or the use of several learners. Ma and Xia [20]  
204 presented a tribe competition-based genetic algorithm for FS in pattern  
205 classification to obtain an optimal feature subset and produce more accu-  
206 rate classifiers. Wei et al. [21] developed a binary particle swarm optimiza-  
207 tion (BPSO) with SVM based on memory renewal and enhanced mutation  
208 mechanisms for FS. Perez-Rodriguez et al. [22] demonstrated that using  
209 evolutionary computation for simultaneous instance and feature selection  
210 plus feature weighting can improve model accuracy significantly. Huang  
211 and Chang [23] proposed GA for FS and HO a SVM in microarray clas-  
212 sification. Ding [24] used PSO in hyperspectral classification of remote  
213 sensing images. Vieira et al. [25] employed a binary PSO with a wrap-  
214 per SVM approach to predict survived or deceased patients with septic  
215 shock. Huang and Dun [26] designed a distributed PSO for FS and HO.  
216 Wan et al. [27] presented a modified binary coded ant colony optimization  
217 algorithm combined with genetic algorithm for FS. Ahila et al. [28] used  
218 PSO for classification of power system disturbances. Dhiman et al. [29]  
219 proposed a hybrid approach with a GA-SVM scheme for FS and HO in  
220 detecting epileptic seizures from background electroencephalogram sig-

221 nals. Winkler et al. [30] reported a variety of evolutionary strategies to  
222 optimize different machine learning models in the identification of tumor  
223 markers. Wang et al. [31] performed HO and FS in medical diagnoses with  
224 a chaotic moth-flame optimization strategy. Medjahed et al. [32] proposed  
225 the use of a gray wolf optimizer in hyperspectral image classification.

226 In general, these works use a more or less complex fitness function, but  
227 they only include a regularization mechanism in the training algorithm  
228 and not in the whole wrapper model selection process. Few method-  
229 ologies search the best parsimonious solution based on minimizing the  
230 cost and complexity of the whole wrapper. Chen et al. [33] used an  
231 evolutionary approach to simultaneously reduce complexity and optimize  
232 weights of learning vector quantification networks for bankruptcy predic-  
233 tion. Avalos et al. [34] presented a methodology based in two penalization  
234 schemes, PAM1 and PAM2, for carrying out both function estimation and  
235 variable selection to obtain parsimonious additive models (PAM). Escobar  
236 and Morales-Menendez [35] developed a penalized maximum probability  
237 of correct decision (PMPCD) model selection criterion to efficiently solve  
238 the trade-off between  $N_{SF}$  and prediction in an ultrasonic metal welding  
239 quality control application. With this methodology, selected parsimonious  
240 model had only 4 inputs from a highly unbalanced database formed by 54  
241 features.

### 242 2.3. Searching parsimonious solutions with GA-PARSIMONY

243 Small differences in the cost can be superfluous in many real appli-  
244 cations. For example, researchers looking for a model that predicts the  
245 temperature set points (within 700-1000°C) of a steel furnace prefer robust

246 solutions with few inputs rather than marginal reductions of the cost. A  
 247 difference between two models below  $\pm 1^\circ\text{C}$  can be insignificant. How-  
 248 ever, obtaining a parsimonious solution with high accuracy can be very  
 249 useful to mitigate the uncertainty caused by perturbations in the produc-  
 250 tion lines, such as noise and the tolerance of sensors. Simpler models are  
 251 also easier to implement, update and understand.

252 For this purpose, Sanz-Garcia et al. [11] presented GA-PARSIMONY,  
 253 a SC methodology based on GA to search accurate parsimonious mod-  
 254 els. This SC method optimizes a KDD-wrapper scheme with GA by using  
 255 a parsimonious model selection (PMS). In each GA generation, the best  
 256 solutions are first sorted by their cost ( $J$ ), and then individuals with less  
 257 complexity are moved to the top positions when the absolute difference  
 258 between their  $J$ s is lower than a threshold value ( $\alpha$ ). Therefore, the se-  
 259 lection of less complex solutions among those with similar accuracy pro-  
 260 motes the evolution of robust models with better generalization capabili-  
 261 ties. Another advantage of this methodology is that it eliminates the use  
 262 of the regularization penalty weight  $\lambda$  because complexity and cost are  
 263 evaluated separately.

264 Figure 4 shows an example of how the selection process of GA-PARSIMONY  
 265 works with four individuals and  $\alpha = 1$ . The process begins by defining  
 266 an initial population of chromosomes  $\Lambda_0 : \{\lambda_0^1, \lambda_0^2, \dots, \lambda_0^P\}$  using a Latin  
 267 Hypercube Sampling (LHS()):

$$\Lambda_0 : \{\lambda_0^i, i = 1, \dots, P\} \leftarrow LHS() \quad (6)$$

268 where  $\lambda_0^i$  is the  $i$  chromosome of the first generation ( $g = 0$ ) and  $P$  is  
 269 the number of individuals. The maximum number of generations ( $G$ ), the

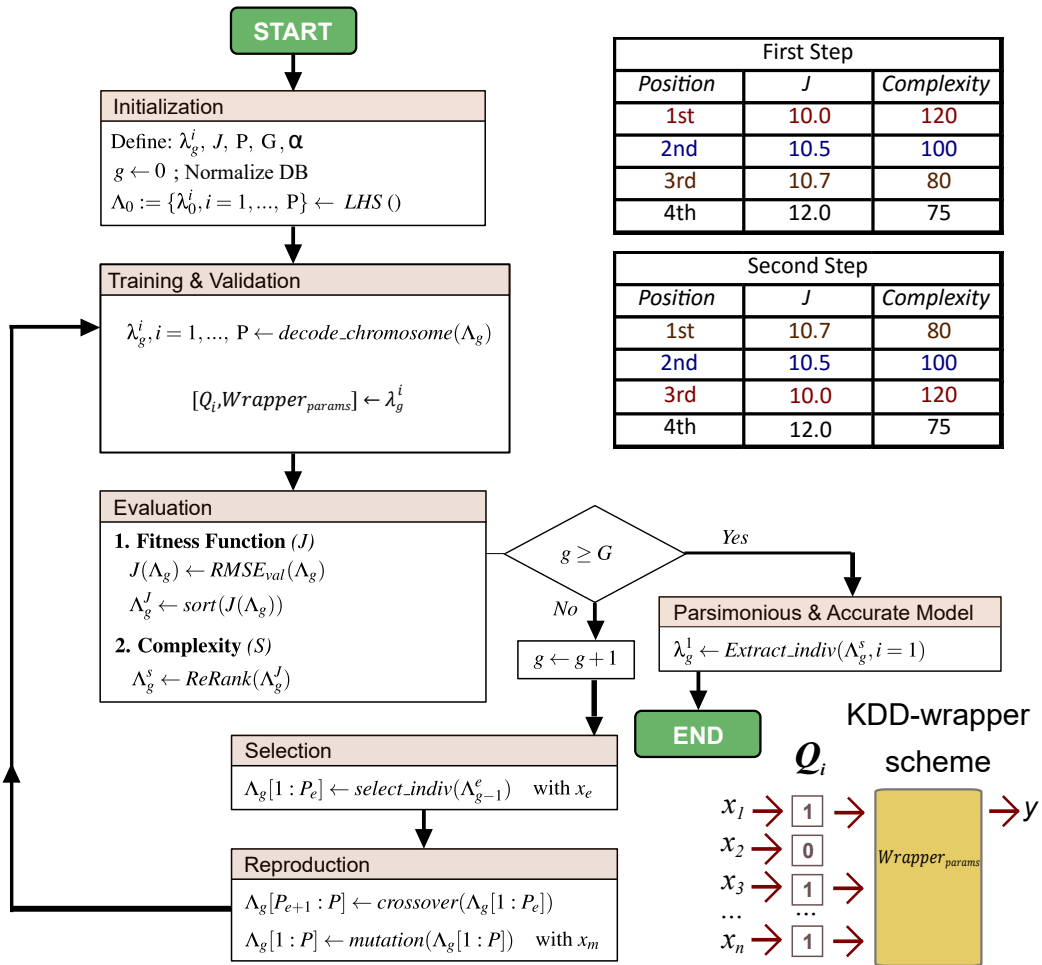


Figure 4: Flowchart of GA-PARSIMONY with a little example how the selection process works for four individuals with  $\alpha = 1$ .

270 cost function ( $J$ ) and  $\alpha$  have to be defined as well. Each chromosome  $i$   
271 composed by two parts: (i) a binary coded array ( $Q_i$ ) that represents the  
272 inputs used, and (ii) the parameters of the wrapper model being optimized  
273 ( $Wrapper_{params}$ ) (Eq. 7).

$$\lambda_g^i = [Q_i, Wrapper_{params}] \quad (7)$$

274 The evaluation and selection processes consist on a separated evalu-  
275 ation of cost and complexity. Following the example of temperature set  
276 points, in the first step, individuals are sorted by their  $J$ , which is ob-  
277 tained with the Root Mean Squared Error (RMSE) using repeated cross-  
278 validation. Differences smaller than  $1^\circ\text{C}$  are considered not significant.  
279 Therefore, in the second step, individuals are rearranged by their *Complex-*  
280 *ity* if the difference between their  $J$ s is lower than  $\alpha = 1.0$ . Consequently,  
281 the parsimonious individual with  $Complexity = 80$  and a difference with  
282 the lowest  $J$  of 0.7 is moved to the first position.

283 GA-PARSIMONY has been successfully applied with support vector  
284 regression (SVR), random forest (RF), ANN and GBM in a wide range of  
285 fields such as solar radiation forecasting [36], industrial processes [37] or  
286 hotel room demand estimation [38]. Besides, GA-PARSIMONY has been  
287 already used for predicting the force-displacement of bolted components  
288 [10]. In that study, GA-PARSIMONY was used to optimize the search of  
289 parsimonious SVR models for seven key parameters of the curve. The SC-  
290 based models reported a high degree of accuracy with new predictions.

#### 291 2.4. *Ensembled methods for reducing bias and variance*

292 Ensemble methods (EM) combine multiple models into one more accu-  
293 rate than the best of them. EM are useful when the predictive accuracy of  
294 the problem is more important than model interpretability. Bagging [39] is  
295 one of the most popular methods among some classic EM such as Random  
296 Forest (RF), AdaBoost, Stacking or Gradient Boosting Machines (GBM). It  
297 consists of creating  $n$  base models with different random samples obtained  
298 with replacement from the original dataset. The response is calculated by  
299 averaging the fitted learners, for regression problems, or with the plural-  
300 ity vote or the mean of probabilities, for classification. The advantages of  
301 bagging [13] are that it reduces the test error by smoothing out variance  
302 leaving the bias unchanged, it does not over-fit the data when the number  
303 of base models increase significantly, and it is easily parallelizable.

304 Stacking, also called meta ensembling or stacked generalization, is an-  
305 other well-known method used to minimize the generalization error rate  
306 by deducing biases of the generalizers [40]. It combines the outputs of  
307 multiple predictive models (level-0 base models) as training data for an-  
308 other model (level-1 stacked model) to approximate the same target func-  
309 tion. The second level model knows where each base learner performs  
310 better giving an improved prediction accuracy [41]. This meta-model can  
311 be also extended to 3 or more levels, with level- $n$  models learning from  
312 level  $(n-1)$ . The main improvement occurs when there is a high diver-  
313 sity between the base model predictions [42]. Therefore, the second level  
314 model can improve the learning process when several algorithms are used  
315 to construct level-0 models because they provide different points of view



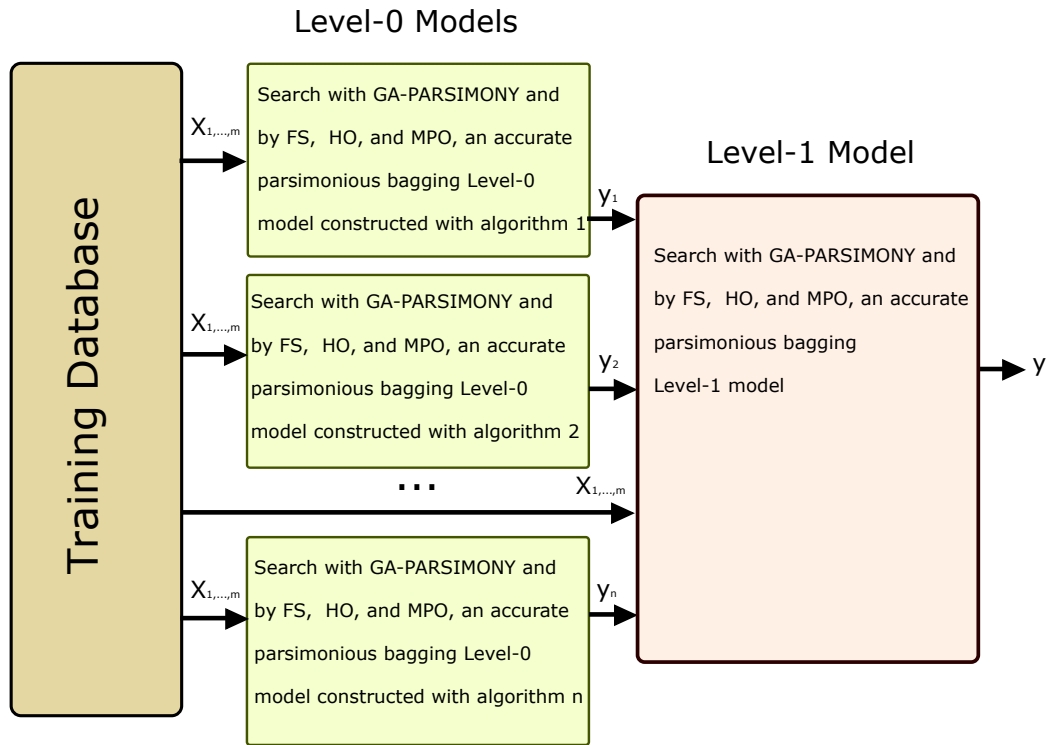


Figure 5: Meta ensemble model constructed with  $n$  parsimonious bagging models in the first level, and a second level parsimonious model which learn from original database and predictions of level-0 base learners. Each parsimonious model are performed with GA-PARSIMONY by optimizing FS, HO and MPO.

316 of the problem.

### 317 3. Stacking ensemble model with GA-PARSIMONY

318 Despite the reasonable prediction capability of SVR models in the char-  
 319 acterization of steel bolted components [10], more accurate tools are re-  
 320 quired to deal with the demanding quality requirements of structural de-  
 321 sign. Therefore, a stacking ensemble model constructed with parsimo-  
 322 nious solutions and different algorithms has been considered in this study.

323 The stacking structure is showed in Figure 5. The basic idea is to com-  
324 bine parsimonious models of different types in a unique meta-learner to  
325 increase diversity and minimize the generalization error rate. First level is  
326 formed by  $n$  parsimonious models created with different algorithms: lin-  
327 ear ridge regression, multilayer perceptron, regression tree, support vector  
328 regression, etc. In order to reduce variance and hence smooth the general-  
329 ization error rate of the base learners, a bagging model is created with each  
330 algorithm. Then, level-1 model use the predictions of base models plus the  
331 original database to reduce biases and improve accuracy. This stacking ap-  
332 proximation is called *Restacking* because it considers not only the outputs  
333 of previous models, but also the original database as inputs. Besides, the  
334 search of good accurate parsimonious bagging models is performed with  
335 GA-PARSIMONY by optimizing feature selection (FS), hyper-parameter  
336 optimization (HO) and model parsimonious selection (MPO). Therefore, a  
337 robust and reliable model is obtained for each algorithm and level.

338 In order to avoid leaking in the training process, the stacked generaliza-  
339 tion method with GA-PARSIMONY is based on a nested cross-validation  
340 scheme (see Fig. 6). A training dataset is divided in  $n$  outer folds. For  
341 each  $i$  outer fold, the best parsimonious model (OF- $i$  model) is constructed  
342 with the other  $n-1$  outer folds by using GA-PARSIMONY. The evaluation  
343 of each individual in the GA selection is performed with an inner  $k$ -fold  
344 cross-validation (CV) process. Finally, we use the best OF- $i$  model to pre-  
345 dict the response for the  $i$  outer fold. The response with a new dataset can  
346 be also obtained with the average of the  $n$  OF-models predictions.

347 Fig. 6 shows an example of how a nested cross-validation scheme works

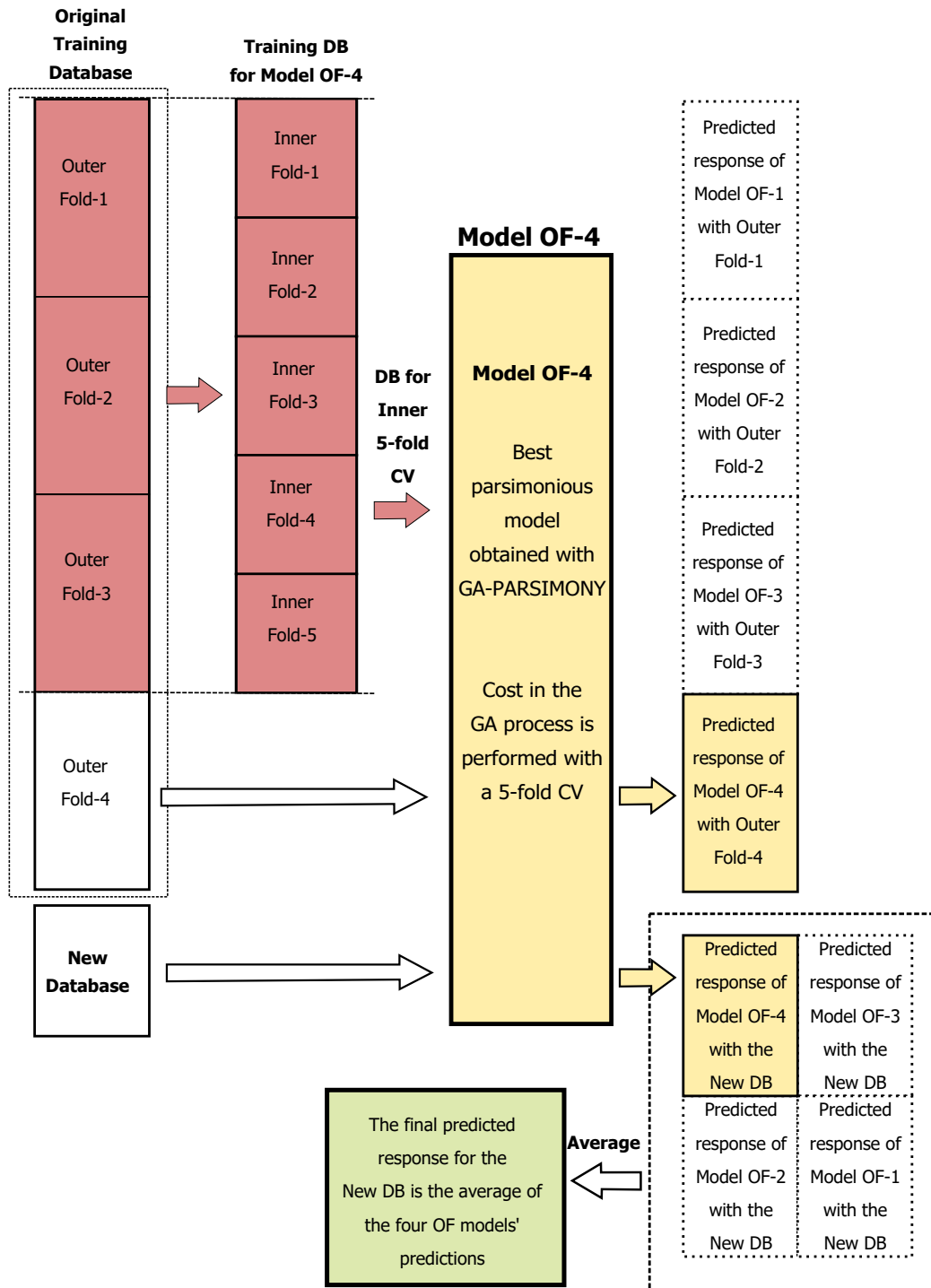


Figure 6: Example of the search for the best parsimonious model for outer fold-4 and using GA-PARSIMONY with a nested cross-validation process with 4 outer folds and 5 inner folds.

348 for  $n = 4$  and  $k = 5$ . In this case, the training database is divided in  $n = 4$   
349 outer folds. For the  $i = 4$  outer fold, GA-PARSIMONY method is used  
350 to search for the best parsimonious OF-4 model by FS, HO and PMS, and  
351 with a dataset created with the 1, 2, and 3 outer folds. Evaluation of the  
352 best individuals in the GA process is performed with this dataset and a  
353  $k = 5$  inner CV. When the GA optimization process ends, the best parsimonious  
354 OF-4 model is used to predict the response for the outer 4-fold  
355 and also, for the new database. At the end of the process, the predictions  
356 for all outer folds are obtained and four predictions for the new database  
357 that can be averaged into a single response.

358 The process can be carried out with each algorithm (ANN, CUBIST,  
359 SVR, GBM, Ridge Linear Regression, etc.) but the following settings must  
360 be defined before using GA-PARSIMONY:

- 361 •  $\alpha$ , which is the maximum absolute difference between two model  
362 costs ( $J$ ) to be considered similar.
- 363 • A complexity function which measures the model parsimony.
- 364 • The ranges of the parameters that need to be tuned.
- 365 • GA settings: number of individuals per population, maximum of  
366 generations, percentage of elitism and mutation, etc.

367 Once the best parsimonious models have been created, the second step  
368 is to build the stacking ensemble model (Fig. 7). Our proposal creates a  
369 new training database by combining the original one and the response pre-  
370 dictions with each OF- $i$  model and for each  $i$  outer fold. Furthermore, the

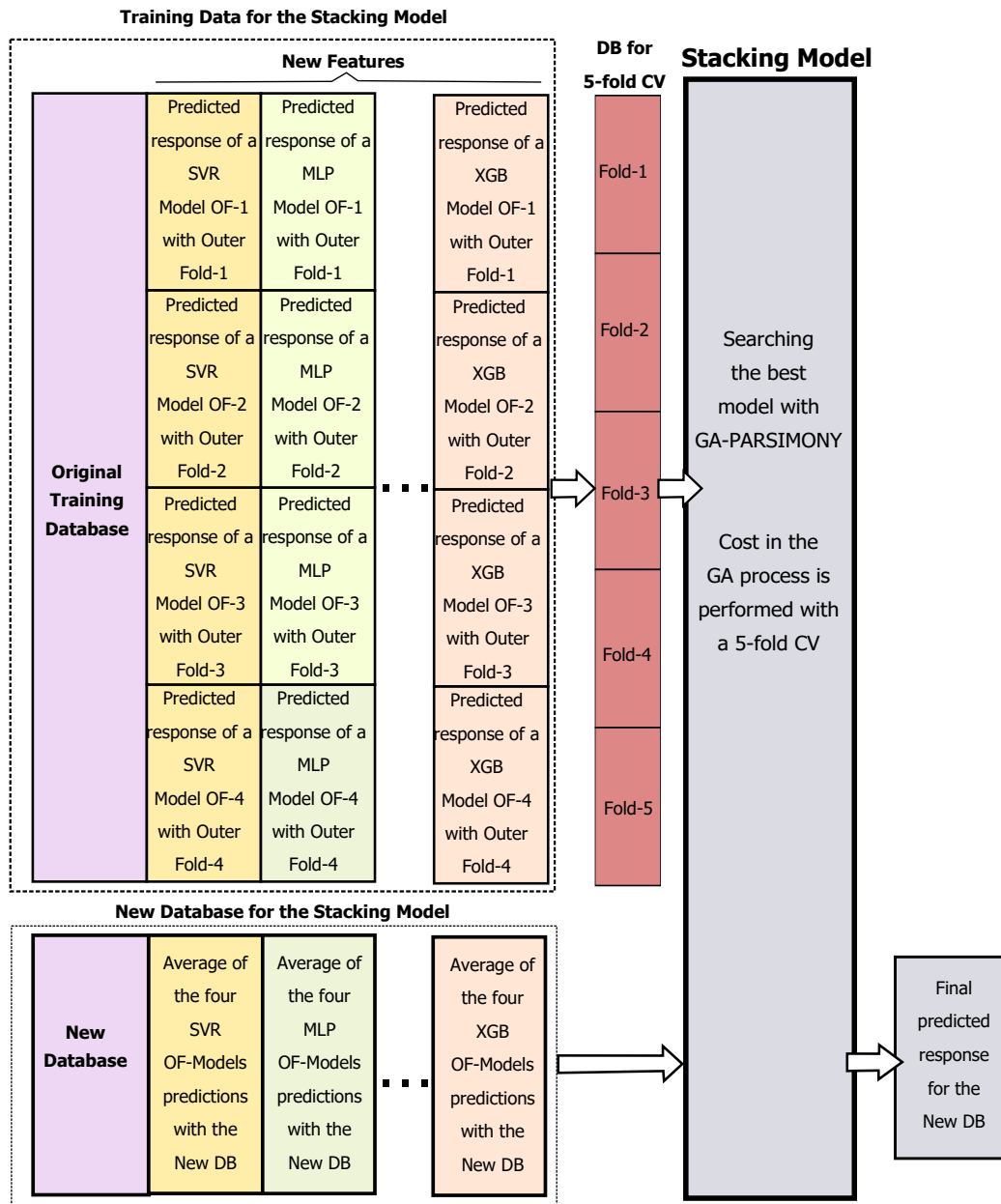


Figure 7: Stacking ensemble model with a training dataset built with the original datasets plus the predictions of best parsimonious models created with different algorithms and using GA-PARSIMONY.

371 new database is constructed in the same way. Finally, a stacking ensemble  
372 model is created with this training database and using GA-PARSIMONY  
373 with a robust machine learning algorithm.

## 374 **4. Experiments**

### 375 *4.1. T-stub component and FE model*

376 The T-stub component comprises two t-shape profiles tied by their  
377 flanges with one or more bolt rows (Fig. 1b) [43]. The tensile load applied  
378 to the web is transferred by the flange in bending and the bolts in tension.  
379 During this process, the contact between flanges produces a prying action  
380 that increases the forces developed in the bolts. The contact area, as well  
381 as the pressure magnitude, evolves during the loading process, render-  
382 ing an adequate evaluation of the force-displacement response difficult.  
383 Non-linear material laws, large deformations and the existence of differ-  
384 ent failure patterns also represent significant sources of complexity in the  
385 calculation of the T-stub component.

386 Numerical approaches such as the FE method constitute a reliable tool  
387 for assessing steel connections. An advanced FE model of the T-stub com-  
388 ponent is described in detail by the authors in [44]. The FE model includes  
389 complete stress-strain nonlinear material relationships and a refined char-  
390 acterization of the bolt, including threaded length, nut and washers (Fig. 8a).  
391 Additionally, the main novelty of the numerical model is the implemen-  
392 tation of a continuum damage mechanics model to simulate the failure of  
393 the bolted connection. Thus, the force-displacement response of the T-stub  
394 can be fully characterized, from the initial stiffness up to the fracture point

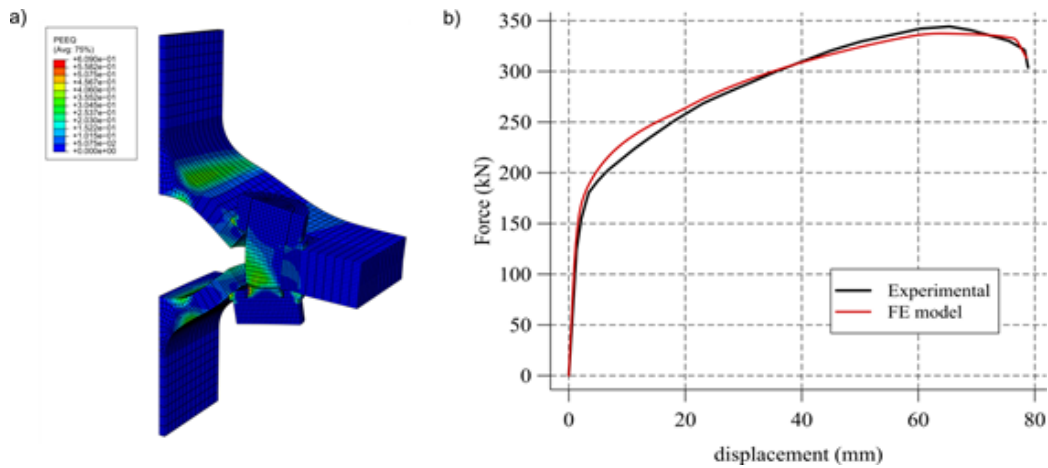


Figure 8: Advanced FE model of the T-stub bolted component [44]. a) FE simulation: equivalent plastic strain (PEEQ); b) Force-displacement response: FE model vs. experimental test.

395 (Fig. 8b).

#### 396 4.2. Generation of the training and test dataset with Design of Computer Experiments 397 *iments*

398 Design of Computer Experiments (DoCE) accounts for the determinis-  
399 tic nature of computer experiments assuming that numerical noise is neg-  
400 ligible. For these cases, space-filling sampling techniques are appropriate  
401 because they uniformly distribute the points over the entire design space.

402 One of the most widely used space-filling designs is the Latin Hyper-  
403 cube Sampling (LHS) [45]. LHS divides each input into  $n$  equally probable  
404 intervals and selects a random value in each interval. The principal advan-  
405 tage of this method is that each input variable is represented in every di-  
406 vision of its range [46]. These space-filling designs are especially useful in  
407 conjunction with non-parametric metamodeling techniques, as employed

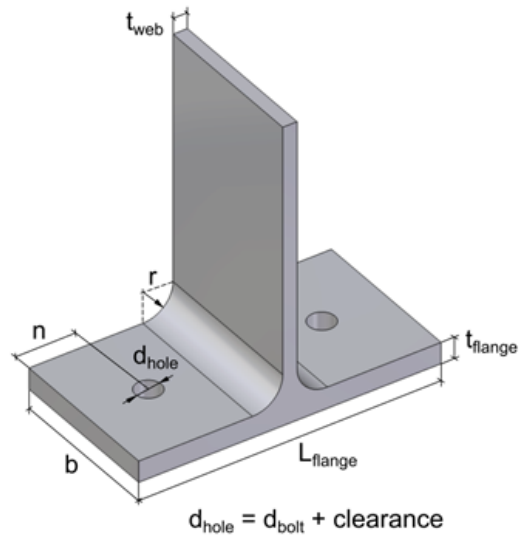


Figure 9: T-stub geometry.

408 in this study.

409 The primary goal of the DoCE is to gain as much information as possible using the minimum number of sample points. However, determining sample size still remains a challenge for practitioners. This parameter relies mainly on the complexity and nonlinearity of the function to be approximated, the dimensionality of the problem, and the modeling technique selected.

415 To create the training dataset, the LHS method was used to define the input values of 820 FE simulations experiments. This number was experimentally determined by prior research [44]. Additionally, two test datasets composed of 76 samples were generated separately so as to check the accuracy and generalization capacity of meta-models in the prediction of unseen data, but also, one of them was used to select the best  $\alpha$  parame-



Table 1: Ranges of the input features included in the DoCE.

Variable	Description [units]	Range
$d_{bolt}$	Nominal bolt diameter [-]	[M12 - M27]
$clearance$	Difference between bolt hole and bolt diameter [mm]	[0.50 - 3.50]
$t_{flange}$	Flange thickness of the T-shape profile [mm]	[8.00 - 30.00]
$t_{web}$	Web thickness of the T-shape profile [mm]	[5.00 - 20.00]
$L_{flange}$	Flange length of the T-shape profile [mm]	[52.00 - 180.00]
$r$	Flange-to-web connection radius [mm]	[9.75 - 43.00]
$n$	Dist. from center of bolt hole to flange's free edge [mm]	[15.75 - 106.00]
$b$	Width of the T-shape profile [mm]	[42.00 - 187.00]
$L_{thread}$	Thread length of the bolt [mm]	[2.50 - 60.25]
$\sigma_y$	Yield strength of the structural steel [MPa]	[200 - 400]
$\sigma_u$	Stress at the maximum tensile load of the structural steel [MPa]	[300 - 800]
$E_h$	Strain-hardening coefficient of the structural steel [MPa]	[1000 - 3000]
$\sigma_{yb}$	Yield strength of the bolt steel [MPa]	[640 - 1098]
$\sigma_{ub}$	Stress at the maximum tensile load of the bolt steel [MPa]	[800 - 1200]
$\epsilon_{ub}$	Strain at the maximum tensile load of the bolt steel [-]	[0.07 - 0.14]

421 ter. Therefore, for each combination of input values, a FE simulation was  
422 conducted to characterize the response of the T-stub component. Regarding  
423 the outputs, the performance of meta-models was evaluated for their  
424 prediction of three key parameters of the force-displacement curve: ini-  
425 tial stiffness ( $k_i$ ), maximum strength ( $F_u$ ) and displacement at failure ( $d_f$ )  
426 (Figure 1c).

427 Table 1 describes the feasible ranges of geometrical parameters and me-  
428 chanical properties of hot-rolled profiles and bolts used herein. A graphi-  
429 cal description of the T-stub geometry is also included in Fig. 9.

#### 430 4.3. Regression techniques

431 Once the training and test dataset was generated, the next step was to  
432 create the most parsimonious solutions to be included in the first level of  
433 the stacking ensemble model. In this study, six popular regression algo-  
434 rithms were selected:

- 435 • Linear ridge regression (LIN) [47].
- 436 • Model tree algorithm (CUBIST) which is based on Quinlan’s M5 model  
437 tree [48] and uses a separate-and-conquer strategy to create a tree  
438 with linear models in each leaf.
- 439 • Instance-based learning (KNN) method [49] which is a popular  $k$ -  
440 nearest neighbors regressor.
- 441 • Single-hidden-layer artificial neural network (ANN) [50] with Broyden-  
442 Fletcher-Goldfarb-Shanno (BFGS) training algorithm and weight de-  
443 cay.

Table 2: Range of the parameters for the regression techniques.

Algorithm	Parameter Description	Range
LIN	<i>Ridge</i> - Regularization parameter	[0.00000001 - 0.99999999]
CUBIST	<i>committe</i> - Number of boosting committes	[1 - 20]
	<i>neighbors</i> - Number of neighbors in prediction	[1 - 9]
IBK	<i>k</i> - Number of nearest neighbours	[1 - 40]
	<i>distW</i> - Type of distance weighting	[0=No, 1=1/dist 2=1-dist]
ANN	<i>n</i> - Number of hidden neurons	[1 - 25]
	<i>decay</i> - Weight decay	[0.0001 - 0.9999]
	<i>maxit</i> - Maximum number of iterations	1000
SVR	<i>C</i> - Error penalty coefficient	$10^{[-3.9] - 2.5}$
	$\gamma$ - Parameter of the RBF kernel	[0.000001 - 0.999999]
	$\epsilon$ - Insensitive loss parameter	[0.000001 - 0.999999]
XGB	<i>max_depth</i> - Max. depth of a tree	[1 - 3]
	<i>min_child</i> - Min. sum of instance weight in a child	[0.10 - 50.00]
	<i>subsample</i> - Subsample ratio of training instance	[0.50 - 1.00]
	<i>alpha</i> - L1 regularization term on weights	[0.00 - 1.00]
	<i>num_trees</i> - Number of trees	[10 - 2000]
	<i>col_sample</i> - Subsample ratio of columns for split	1.0
	<i>eta</i> - Step size shrinkage in update (learning rate)	0.05

- 444 • Support vector regression (SVR) technique [51] with radial-basis func-  
445 tion (RBF).
- 446 • EXtreme Gradient Boosting (XGB) machines [52] which is based on  
447 gradient boosting machines (GBM) [53].

448 Table 2 shows the ranges of setting parameters included in the GA-  
449 PARSIMONY optimization process.

450 In addition, model complexity was defined as follows:

$$Complexity = 10^6 N_{SF} + C_{mod} \quad (8)$$

451 where  $N_{SF}$  is the number of input selected features and  $C_{mod}$  is the in-  
452 ternal model complexity [54]. This expression gives priority to the  $N_{SF}$   
453 term to penalize individuals with more number of input features. Internal  
454 complexity plays importance when two models have the same number of  
455 inputs. Due to  $N_{SF}$  is weighted with a high value ( $10^6$ ),  $C_{mod}$  is trunked  
456 to a value of 999999 if it exceeds this upper limit. This hybrid complexity  
457 metric has demonstrated good behavior in PMS within previous experi-  
458 ments developed by the authors [11, 36, 55, 37, 38]. The following  $C_{mod}$   
459 metrics were defined for each regression technique:

- 460 • LIN:  $C_{mod} = \sum \beta_i^2$  where  $\beta_i$  are the coefficients of the equation.
- 461 • CUBIST:  $C_{mod}$  corresponds to the mean of the number of trees rules.
- 462 • KNN:  $C_{mod} = (10^6 / K) - 1$  where  $K$  are the number of nearest neigh-  
463 bors.
- 464 • ANN:  $C_{mod} = \sum w_i^2$  where  $w_i$  are the weights of the network.
- 465 • SVR:  $C_{mod}$  corresponds to the number of support vectors.
- 466 • XGB:  $C_{mod} = 10^4 max\_depth$  which depends on the tree depth.

467 Finally, bagging ensemble model with 10 bags was considered to re-  
468 duce variance as base model for each technique: BaggLIN, BaggCUBIST,  
469 BaggKNN, BaggANN, BagSVR, and BaggXGB.

#### 470 4.4. GA-PARSIMONY settings

471 For each  $i$  outer-fold and regression technique, GA-PARSIMONY searched  
472 the best parsimonious OF- $i$  model by validating the individuals with an  
473 inner 5-CV Root Mean Squared Error ( $J = RMSE_{val}$ ). Besides, several ex-  
474 periments were performed with different  $\alpha$  values for each method and  
475 response variable ( $k_i$ ,  $F_u$  and  $d_f$ ), to promote parsimonious solutions into  
476 the PMS process.

477 The GA optimization process was performed with the following set-  
478 tings. A population size of 80 and a maximum number of generations of  
479 100 but with an early stopping strategy when  $J$  of the best individual does  
480 not decrease in 10 generations. Starting with the PMS selection method at  
481 the 10th generation. The mutation percentage was 10% for all individu-  
482 als except the three best elitists of each generation. The elitism percentage  
483 was 20%. The selection method was based on *linear-rank*, *heuristic blend-*  
484 *ing* for parameter crossing [56], and binary random swapping for feature  
485 crossing.

486 All experiments were conducted with the statistical software R [57],  
487 GAparsimony package [58] and nine Intel 24-core servers of Beronia HPC  
488 cluster (Intel ®Xeon ®E5-2670 @ 2.30GHz).

## 489 5. Results

490 Table 3 shows  $J$ , *Complexity*, and the RMSE with a new test dataset  
491 ( $RMSE_{tst}$ ) of the best BaggsVR models for  $d_f$  and different values of  $\alpha$ .  
492 In this table, a clear trend of increasing  $RMSE_{val}$  can be observed when  $\alpha$   
493 grows but, inversely, model complexity decreases when  $\alpha$  is higher. The

Table 3:  $J$ ,  $RMSE_{tst}$  and  $Complexity$  of the best BaggsVR models for  $d_f$  response. Parsimonious models were obtained with GA-PARSIMONY and different  $\alpha$  values for controlling the trade-off between  $J$  and  $Complexity$ .

$\alpha$	$J = RMSE_{val}$	$Complexity$	$RMSE_{tst}$
0	7.699	8 750390.7	6.332
0.001	7.717	8 750353.6	6.315
0.01	7.849	8 500317.0	6.788
0.08	7.707	7 750259.6	6.884
0.1	7.736	7 750209.2	6.170
0.2	7.787	7 500183.8	5.906
0.4	7.880	7 000146.3	5.890
0.7	8.121	7 000108.7	5.783
0.8	8.160	7 000103.0	5.850
0.9	8.413	6 750128.2	6.096
<b>1.0</b>	<b>8.270</b>	<b>7 000099.5</b>	<b>5.765</b>
1.2	9.122	6 750047.5	6.175
1.5	10.403	5 750066.0	7.553
1.7	10.645	5 500047.2	8.396
2.0	10.774	4 750076.4	9.965
2.2	10.657	4 750086.4	10.367
2.5	11.571	4 500056.8	11.610

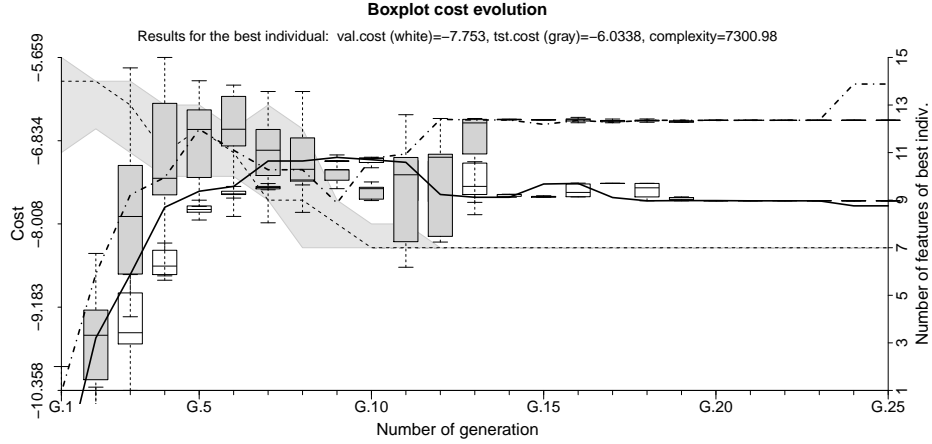


Figure 10: Evolution of the OF-1 BaggsVR models for  $d_f$  and using GA-PARSIMONY with  $\alpha = 1.0$ . White and grey box-plots represent  $RMSE_{val}$  and  $RMSE_{tst}$  elitist evolution, respectively. Continuous and dashed-dotted lines show the  $RMSE_{val}$  and  $RMSE_{tst}$  of the best individual, respectively. The shaded area delimits the maximum and minimum number of  $N_{FS}$ , and the dashed line, the  $N_{FS}$  of the best individual.

494 best trade-off between  $J$  and *Complexity* is achieved with  $\alpha = 1.0$ , re-  
 495 ducing the testing error to 9.83% compared to the best model with Par-  
 496 simony Model Selection (PMS) disabled ( $\alpha = 0$ ). Therefore, the model  
 497 with the best generalization capability is achieved with GA-PARSIMONY  
 498 and  $\alpha = 1.0$ . For this BaggsVR, 7 of 15 initial features are selected, with a  
 499 mean of  $C_{mod} = 99.5$  support vectors of all SVR models. Similar behavior  
 500 can be observed with other algorithms and response variables.

501 Figure 10 displays, for  $d_f$  response, the search of the best parsimonious  
 502 BaggsVR model for the outer-fold 1 (OF-1 BaggsVR) with GA-PARSIMONY  
 503 and  $\alpha = 1.0$ . This figure shows the evolution of negative values of  $J =$   
 504  $RMSE_{val}$  and  $RMSE_{tst}$  (in order to represent the best solutions on the top),

505 and the number of model features selected ( $N_{FS}$ ) of elitists. In this exam-  
506 ple, with  $\alpha = 1.0$ , GA-PARSIMONY starts the PMS method at the 10th  
507 generation to search parsimonious solutions, in spite of getting worse  $J$ .  
508 Therefore, GA-PARSIMONY improves  $RMSE_{tst}$  by reducing model com-  
509 plexity.

510 Table 4 shows the  $\alpha$  value of the bagging model with the best general-  
511 ization capability (best  $RMSE_{tst}$ ) for each algorithm and response variable.  
512  $J = RMSE_{val}$ ,  $RMSE_{tst}$ , and *Complexity* are also presented. The 7th col-  
513 umn corresponds to the relative percentage reduction of  $RMSE_{tst}$  versus  
514 the model selected with PMS of GA-PARSIMONY disabled ( $\alpha = 0$ ). Fi-  
515 nally, the last column presents the total minutes, in a 24-core server, used  
516 to search for the best model with GA-PARSIMONY and with the 17  $\alpha$  val-  
517 ues of Table 3.

518 For the three response variables, BaggANN obtains the best solutions  
519 as compared to the other algorithms. In addition, BaggSVR, BaggCUBIST  
520 and BaggXGB present accurate solutions for  $d_f$ . However, the computa-  
521 tional effort necessary is much greater with these algorithms than com-  
522 pared to the other methods. Moreover, an important improvement in the  
523 generalization capability is achieved with PMS (more than 5%  $RMSE_{tst}$   
524 reduction) in BaggLIN and BaggSVR  $d_f$  models, and in BaggLIN and Bag-  
525 gANN  $F_u$  models. For  $k_i$ , BaggANN and BaggSVR obtain the best accu-  
526 racy, but PMS improves these results slightly.

527 Table 5 presents the final results of the stacking model (StackANN)  
528 that has been trained as explained in Section 3. The training database is  
529 formed by combining the outer-folds responses from the models of Table 4



Table 4: Value of  $\alpha$  to obtain the best GA-PARSIMONY model for each response variable and algorithm. Seventh column shows the percentage of  $RMSE_{tst}$  reduction versus the error of the best model with PMS disabled ( $\alpha = 0$ ). Last column presents the total elapsed time in a 24-core server to search the best model with GA-PARSIMONY and with the 17  $\alpha$  values of Table 3.

Resp.	Algorithm	$\alpha$	$RMSE_{val}$	Complexity	$RMSE_{tst}$	$RMSE_{tst}$ reduction	Total minutes
$d_f$	BaggCUBIST	0.20	7.842	7 000008.2	5.799	3.59%	2605.4
$d_f$	BaggKNN	0.00	12.193	6 258332.3	11.458	0.00%	13.0
$d_f$	BaggLIN	0.20	10.438	7 500001.3	8.397	5.30%	26.8
$d_f$	<b>BaggANN</b>	0.20	6.494	9 500079.9	<b>4.971</b>	2.10%	1750.8
$d_f$	BaggSVR	1.00	8.270	7 000100.0	5.765	9.83%	543.7
$d_f$	BaggXGB	0.20	8.330	8 020000.1	5.989	3.45%	376.5
$F_u$	BaggCUBIST	0.40	17.034	9 500006.1	13.785	4.00%	2393.4
$F_u$	BaggKNN	0.00	48.704	6 454165.8	36.301	0.00%	16.2
$F_u$	BaggLIN	1.70	30.546	7 000000.2	26.362	4.82%	33.9
$F_u$	<b>BaggANN</b>	0.20	11.779	11 750039.1	<b>9.469</b>	8.16%	3215.3
$F_u$	BaggSVR	0.08	16.876	10 250314.9	13.180	1.73%	1174.7
$F_u$	BaggXGB	1.00	21.205	8 767500.0	16.566	2.26%	692.9
$k_i$	BaggCUBIST	0.08	11.279	9 500011.2	10.968	1.80%	3396.6
$k_i$	BaggKNN	0.70	39.641	4 927380.0	34.533	0.32%	14.4
$k_i$	BaggLIN	0.10	25.805	9 250001.0	22.582	0.22%	33.9
$k_i$	<b>BaggANN</b>	0.10	8.243	11 000039.4	<b>7.822</b>	1.46%	3034.1
$k_i$	BaggSVR	0.01	9.603	9 750348.1	8.154	1.21%	1814.3
$k_i$	BaggXGB	0.00	17.146	7 770000.0	16.016	0.00%	929.3

Table 5: Results of the stacking model with PMS (StackANN) versus a stacking model constructed with the same methodology but with PMS disabled ( $\alpha = 0$ ) (Stack\_NOPMS). Results of the best model of the first level are also displayed (BaggANN from Table 4) and of a single SVR developed in previous research [10]. Table presents  $\alpha$  and  $RMSE_{tst}$ . Additionally,  $RMSE$ , and the mean and standard deviation of the squared error with a new second testing dataset ( $tst2$ ) are shown.

Resp.	Algorithm	$\alpha$	$RMSE_{tst}$	$RMSE_{tst2}$	$SE_{tst2}^{mean}$	$SE_{tst2}^{sd}$
$d_f$	<b>StackANN</b>	0.10	<b>4.709</b>	<b>3.681</b>	<b>13.547</b>	<b>29.378</b>
$d_f$	BaggANN(1st level)	0.20	4.971	4.534	20.560	39.934
$d_f$	StackNO_PMS	0.00	5.237	4.166	17.358	36.555
$d_f$	Fernandez-Ceniceros et al. [10]		7.260			
$F_u$	<b>StackANN</b>	0.10	<b>9.031</b>	<b>8.640</b>	<b>74.649</b>	<b>125.840</b>
$F_u$	BaggANN(1st level)	0.20	9.469	9.192	84.493	169.375
$F_u$	StackNO_PMS	0.00	10.486	10.052	101.038	169.788
$F_u$	Fernandez-Ceniceros et al. [10]		15.970			
$k_i$	<b>StackANN</b>	0.08	<b>7.637</b>	<b>5.111</b>	<b>26.118</b>	<b>57.892</b>
$k_i$	BaggANN(1st level)	0.10	7.822	5.204	27.087	69.772
$k_i$	StackNO_PMS	0.00	7.823	5.993	35.922	81.273
$k_i$	Fernandez-Ceniceros et al. [10]		11.750			

530 and the original training dataset. The last three columns correspond to  
531 the errors with a new testing database ( $tst2$ ). Additionally, the  $RMSE_{tst2}$ ,  
532 mean ( $SE_{tst2}^{mean}$ ), and standard deviation ( $SE_{tst2}^{sd}$ ) of the squared error with  
533 this new dataset are included. The objective is to check the models gener-  
534 alization capability with a new database that has not been used to select  
535 the best  $\alpha$ .

536 StackANN corresponds to a stacking parsimonious Bagging ANN model  
537 which has been built with the original database and the predictions of best  
538 base models from level-0, as it has been explained in Section 3. Second line

539 corresponds with the results of the best bagging ANN level-0 model (Bag-  
 540 gANN(1st level) of Table 4). Third line shows errors with the stacking  
 541 bagging ANN model (StackNO\_PMS) constructed with the same method-  
 542 ology, but where all base and second level models were obtained with PMS  
 543 of GA-PARSIMONY disabled ( $\alpha = 0$ ). Finally, results of a previous study  
 544 [10] are presented.

545 The three StackANN models significantly improve errors in both test-  
 546 ing databases versus StackNO\_PMS models. This proves that incorpor-  
 547 ating PMS into the GA-PARSIMONY process helps to obtain parsimo-  
 548 nious models with better generalization capabilities. Moreover, the stack-  
 549 ing method of StackANN improves results for the first level model (Bag-  
 550 gANN) by increasing diversity and reducing the generalization error rate.  
 551 Finally, it can be observed that  $SE_{tst2}^{sd}$  is reduced with StackANN for the  
 552 three response variables. Therefore, the proposed methodology creates  
 553 more accurate, robust, and reliable models thanks to the combination of  
 554 parsimonious base models in the first level.

555 Figure 11 shows error of StackANN model vs the three measured re-  
 556 sponses from test database.  $df$  and  $Ki$  have a normal distribution with the  
 557 median close to 0. Finally, Figure 12 represents relative error in percentage  
 558 that it is defined by:

$$Re_i = 100 \frac{\hat{y}_i - y_i}{y_i} \quad (9)$$

559 This figure highlights the prediction capability for the three output  
 560 variables. These relative errors represent useful information for structure  
 561 designers about the applicability of the proposed model. Regarding the  
 562 prediction of initial stiffness  $k_i$  and maximum strength  $F_u$ , most of the

563 cases were predicted within a scatter band of  $\pm 5\%$ . These results are very  
564 accurate compared with previous models [10] and represent a great im-  
565 provement over analytical models included in current regulatory codes,  
566 such as Eurocode 3.

567 As for the prediction of the displacement at failure  $d_f$ , it presents higher  
568 relative errors, most of them within a scatter band of  $\pm 25\%$ . This lower  
569 prediction capability compared to the other two variables is explained by  
570 the intrinsic randomness of the damage process. The variable  $d_f$  implicitly  
571 accounts for the degradation mechanisms which lead to the failure of the  
572 bolted connection. These mechanisms include very non-linear effects such  
573 as large deformations, necking, nucleation and coalescence of voids, and  
574 can only be predicted by means of advanced FE simulations. Taking all  
575 of this into consideration, the obtained relative errors for this variable are  
576 reasonably accurate. In fact, none of the existing standards and regulatory  
577 codes are able to predict the displacement at fracture, even though the  
578 importance of this variable from the design and safety points of view.

579 Overall, the proposed model represents a powerful tool able to make  
580 predictions on-line and with higher accuracy than current regulatory codes.  
581 This is only possible by the combination of advanced numerical methods  
582 (FEM) to model complex phenomena with SC techniques to alleviate com-  
583 putation burden, as used in this work.

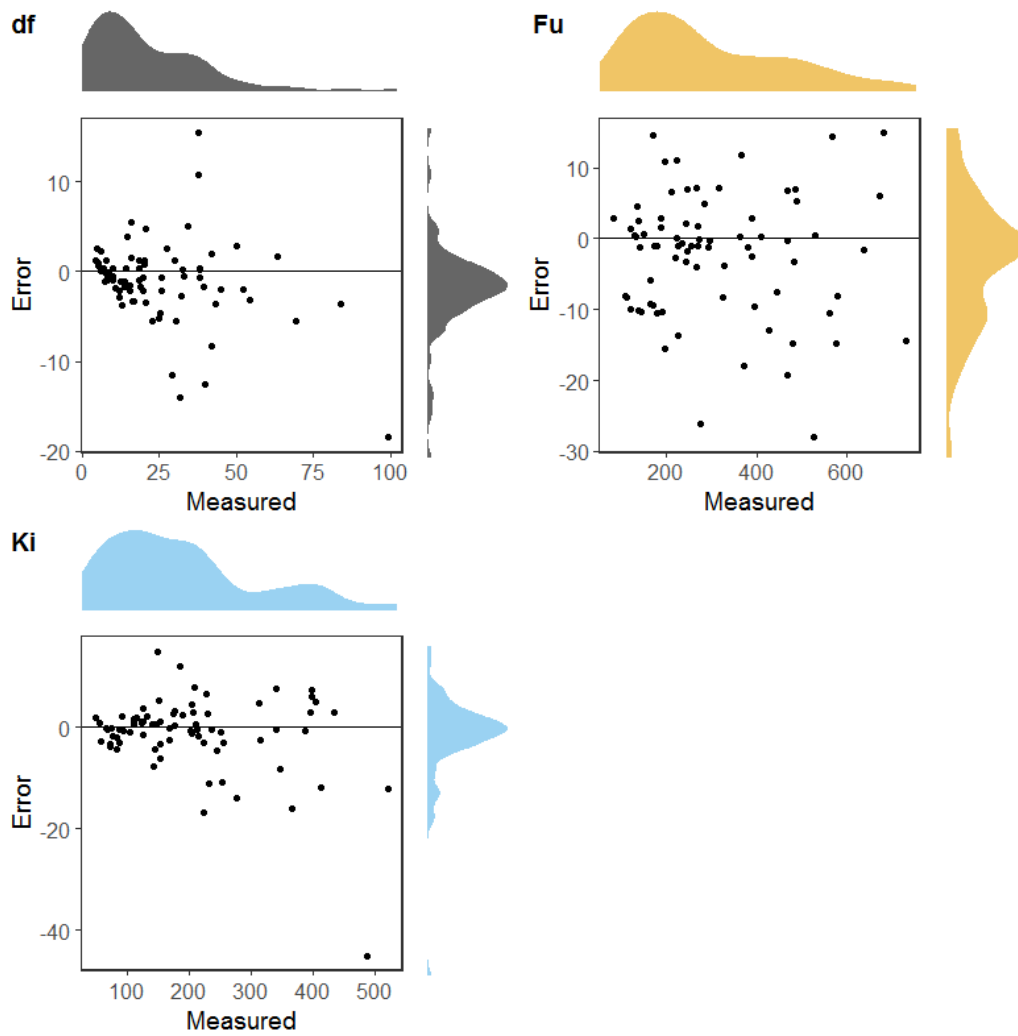


Figure 11: Scatterplot of the errors obtained with StackANN in the test database.

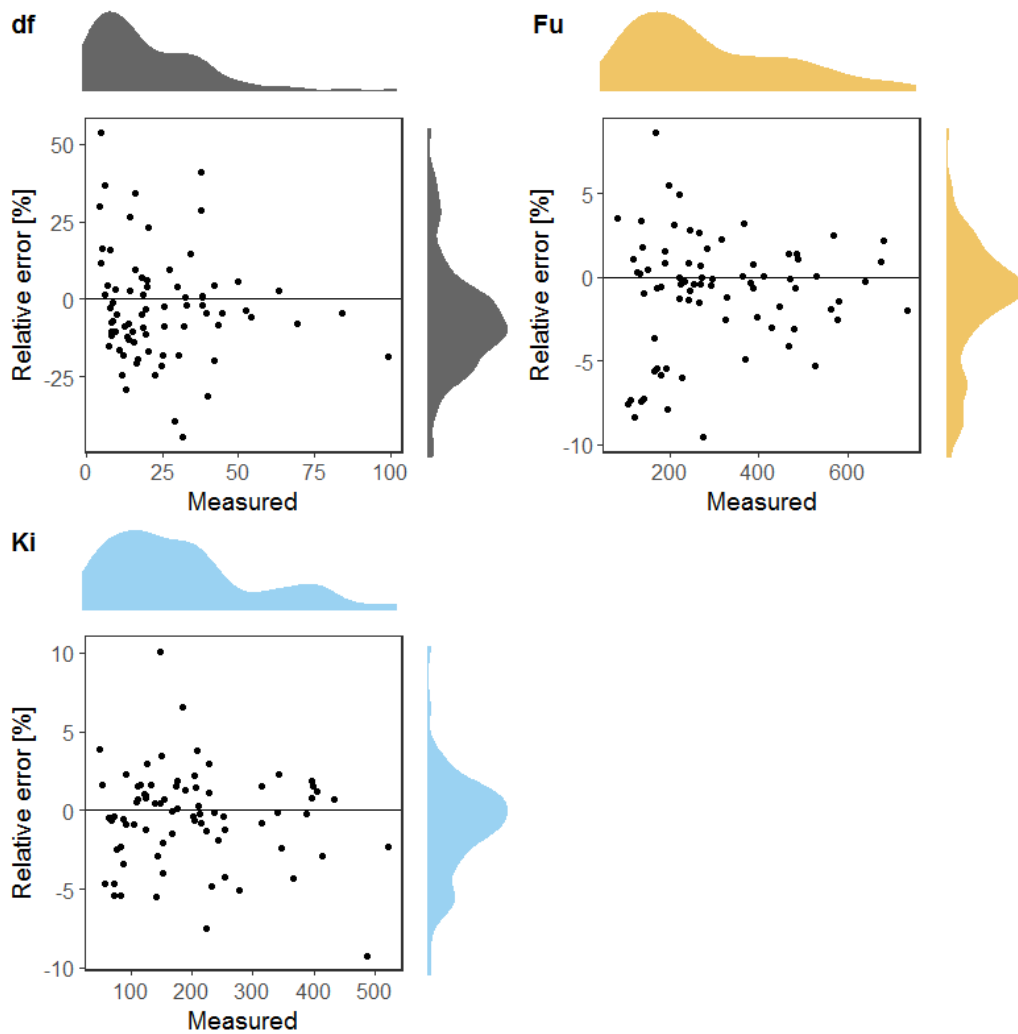


Figure 12: Scatterplot of the relative errors obtained with StackANN in the test database.

584 **6. Conclusions**

585 Current software applications based on machine learning models de-  
 586 mand robust and accurate predictions with unseen new data. Predictions  
 587 of such quality are mandatory in steel structure design from the safety

588 point of view. In particular, in the assessment of steel bolted connec-  
589 tions, the challenge is to create models capable of estimating the force-  
590 displacement responses with great precision and reliability.

591 Today, FEM is one of the most accurate method to predict behavior of  
592 steel bolted components but it is a highly time-consuming process and  
593 hence is inefficient in the design of hundred of joints that form a steel  
594 structure. Thus, the main objective of this work was to create a robust  
595 and accurate meta-model that would be used in real-time within the struc-  
596 tural analysis and desing software. Model learned from a database cre-  
597 ated with FEM simulations that was developed with a Design of Exper-  
598 iments (DoCE) in order to obtain an homogeneous distribution of actual  
599 design solutions. Therefore, this article presents a new methodology for  
600 building robust and reliable models of three key parameters of the force-  
601 displacement curve: maximum resistance, initial stiffness and displace-  
602 ment at failure. The main objective of this study was to develop a robust  
603 stacking ensemble model with parsimonious base models created with dif-  
604 ferent machine learning methods.

605 For this purpose, GA-PARSIMONY, a GA soft computing methodol-  
606 ogy based on feature selection, parameter tuning and parsimonious model  
607 selection was employed. GA-PARSIMONY searched robust and reliable  
608 bagging models with only one tuning parameter,  $\alpha$ , which controls the  
609 trade-off between accuracy and model flexibility. Finally, in order to achieve  
610 greater generalization capability, the best parsimonious models obtained  
611 with different algorithms were combined in a stacking ensemble model by  
612 means of a nested cross validation process.

613 Experiments performed with a small database created with FE simu-  
614 lations demonstrated that the combination of parsimonious models in a  
615 stacking ensemble model improved accuracy with unseen data, against  
616 classical searching methods based on feature selection and parameter tun-  
617 ing.

618 Although, it seems that Stacking with PMS method included in GA-  
619 PARSIMONY could improve generalization capability in applications where  
620 models have to be built from small databases, other experiments will be  
621 necessary to corroborate this conclusion.

622 Finally, this accurate tool could aid the designer to obtain optimized  
623 steel structures. This means less quantity of steel, lighter structures, cost  
624 saving and less embodied CO<sub>2</sub>.

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