Prediction of the Energy Release Rate for Arbitrary Mechanical Properties using Machine Learning for Mode I Deformation

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Structural failure is a common issue in the world of laminated composite materials. To determine failure criteria, it is common to perform failure analyses with the finite element (FE) method along with the J-integral to calculate the energy release rate, G. However, this procedure requires experts in the field of fracture mechanics. Moreover, since a new analysis is required for each composite laminate, the analysis process is time-consuming and may be cumbersome. This study aims to examine the capability and precision of a machine learning (ML) model to predict the energy release rate (ERR) value for arbitrary mechanical properties. By doing so, the FE failure analysis process may be shortened or avoided.

Each composite laminate is composed of several plies stacked together in a specific order resulting in specific mechanical properties. Each ply within the laminate may be mechanically defined. The ply properties are determined based on the type of fibers, their orientation, and the matrix type used in each ply. In addition, it may be noted that for two separate plates of the same laminate, the mechanical properties of each ply may vary by $\pm 15\%$. A reason for this may be the partial hand manufacturing process of the composite. When using FE to analyse failure, the influence of the mechanical properties on the failure characteristics is to be evaluated. This may be performed with additional FE analyses (FEAs) or with a sensitivity study. Whereas, ML algorithms (MLAs) may quantify the dominant properties that most influence the failure characteristics.

For simplicity of the case studied here, a data set was constructed for a specific composite layup and test setup. An FE model of a double cantilever beam (DCB) specimen, illustrated in Fig. 1, was considered. Note that, this model results in nearly pure mode I deformation, namely, nearly pure delamination opening. The layup included three-ply types: a unidirectional (UD) ply with fibers oriented in the $0°$ - direction, and two differently oriented woven plies with tows oriented in the $0°/90°$ or $+45°/-45°$ - directions. Note that a UD ply is considered transversely isotropic defined by five independent effective mechanical properties. A woven ply is considered tetragonal and requires six independent properties to be fully defined. To define all properties in the composite, 17 properties were used. Initial delamination was introduced between an upper UD ply and a lower $+45°/-45°$ woven ply. The constructed data set included the energy release rate that was computed with the J-integral for various sets of properties employed in the FEA. The obtained data set was used for ML training.

A variety of regression MLAs including K nearest neighbours (Knn), support vector machine (SVM), and XGBOOST were employed to predict the ERR as a function of the 17 given properties. These models were chosen since they are not affected by high multicollinearity. Hence, although the 17 mechanical properties have a high VIF score (which indicates high multicollinearity), there is no need to eliminate features from the model. Note that this is essential in the case examined since the model construction purpose is to replace the original numerical FE model used for failure analyses. Hence, including all data input, as employed in the original FE numerical model, is important.

Predictions from these MLAs were compared. Out of the various algorithms evaluated, the highest performing model was XGBOOST, which had the lowest RMSE and the highest R^2 of 1.24 and 0.99, respectively. In addition, this algorithm presented high scores in the Cross-Validation (CV) R^2 & CV R^2 standard deviation (STD) of 0.956 and 0.057, respectively. In Tables 1 & 2 predictions and results from the three MLAs employed are presented for four sets of mechanical properties. These properties were obtained from Mega (2021) for a composite laminate. The obtained ERR predictions are compared with the J-integral values obtained based on FEAs for the same material properties. From the comparison presented in Tables 1 & 2, it may be observed that the best predictions were made by the Knn and XGBOOST models. We find this result to be interesting to fellow researchers in this field as one model is distance-based while the other is tree-based, which define their classification rules in very different manners.

Figure 1: Illustration of a double cantilever beam specimen with specified boundary conditions.

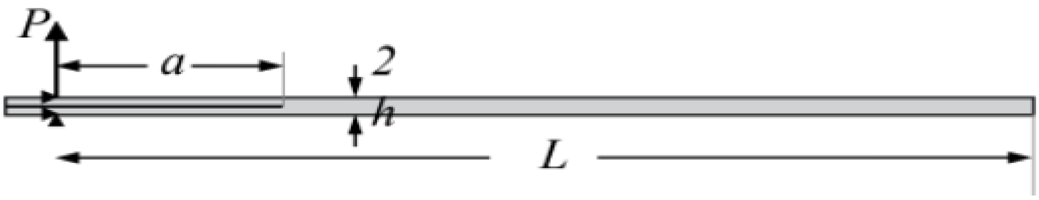

Table 1 : The error from the prediction for known new materials data

Material type (Mega, 2021)	number of properties out of training range	Model Type		
		XGBOOST	**SVM**	**Knn**
Compressed	5	22.909	-595.428	25.711
Expanded	7	-108.251	-511.005	-105.449
Calculated	8	11.993	-632.498	14.794
Used (in range)	0	-2.307	-612.871	0.495

Table 2 : Root mean square error (RMSE) of the models

Models	**RMSE**
XGBOOST	55.660
SVM	589.772
Knn	54.772

References

M. Mega, Mixed mode fracture behavior of a multi-directional laminate composite produced by a wet-layup, *Ph.D. thesis*, Tel Aviv University, Israel (2021).