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Evaluating the impact of 3D constitutive models on predictive performance of xgboost for material parameter identification

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Abstract. This study explores the impact of different 3D constitutive models on the predictive performance of machine learning algorithms, focusing on eXtreme Gradient Boosting (XGBoost) for material parameter identification. Early work with the Hill’48 yield criterion demonstrated strong predictive performance. However, more advanced criteria, such as the yield criterion developed by Cazacu, Plunkett and Barlat (CPB’06), have posed challenges, significantly degrading the machine learning model's performance. The study highlights the need to address the interaction between constitutive models and machine learning methods in material parameter identification. XGBoost models were trained using material datasets generated from biaxial tensile tests on a cruciform sample with the Hill'48 and CPB’06 yield criteria to compare their influence on predictive performance. The poor performance obtained with the latter yield criterion highlights the need for optimized training strategies or potentially larger, more diverse datasets when dealing with complex constitutive models.

Introduction

Accurately predicting the mechanical behavior of materials under complex loading conditions is essential for optimizing sheet metal forming processes. Numerical simulations, combined with advanced constitutive models, play a critical role in capturing the anisotropic and hardening behavior of metallic materials. Among these models, Hill’48 and CPB’06 yield criteria can be used for describing orthotropic plasticity, each offering distinct advantages and challenges due to their mathematical formulations and parameter requirements [1, 2]. Machine Learning (ML) regression techniques, such as those based on XGBoost [3], have emerged as powerful tools for calibrating material parameters from experimental or simulated data, enabling faster and more efficient parameter identification. However, the predictive performance of ML models depends heavily on the complexity of the yield criterion and the quality and quantity of training data available. Early work with XGBoost and Hill'48 yield criterion demonstrated strong predictive performance [4].

This study investigates the performance of Extreme Gradient Boosting (XGBoost) ML models in predicting material parameters for two case studies: Hill’48 (Case Study 1) and CPB’06 (Case Study 2). A biaxial tensile test on a cruciform sample is employed as the mechanical testing approach, generating heterogeneous stress and strain fields representative of real-world forming conditions. The study further explores the impact of training dataset size on prediction accuracy, revealing differences in model sensitivity to data availability and yield criterion complexity. While a 2D anisotropic yield criterion is computationally efficient and often sufficient for biaxial tensile tests, a 3D yield criterion was chosen to account for potential out-of-plane effects and ensure broader applicability. The findings provide valuable insights into the applicability and limitations of ML-based parameter identification for different constitutive models, contributing to more efficient and reliable material behavior predictions in industrial applications.

3D numerical model

This study utilizes a biaxial tensile test on a cruciform sample as the selected mechanical testing approach. The sample's geometry, previously designed in earlier work [5], promote heterogeneous stress and strain fields, capturing a wide range of stress and strain paths commonly observed in sheet metal forming processes. The sample's geometry and in-plane dimensions are illustrated in Fig. 1. To optimize computational efficiency, and due to symmetries in the boundary conditions, sample geometry, and material behavior, the numerical simulation considers only one-eighth of the sample. In fact, the highlighted grey region in Fig. 1 presents symmetry across the three orthogonal planes: $x = 0$ mm, $y = 0$ mm, and $z = 0$ mm. Displacement boundary conditions ensure uniform displacements ($u_x = u_y = 2$ mm) at the ends of both sample arms. The numerical model employs a structured mesh comprising 564 C3D8R elements, characterized by trilinear shape functions and reduced integration. Finite Element Analysis (FEA) simulations are conducted using ABAQUS CAE software [6], with each simulation divided into twenty equally spaced time-steps. Throughout these steps, the forces along the *0x* and *0y* directions, as well as the strain field components (ε_x, ε_y, and ε_{xy}), are recorded at every interval.

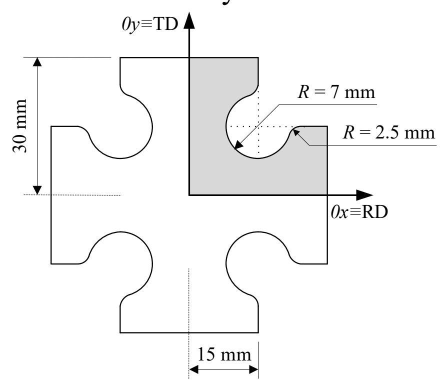

Figure 1 – Geometry and dimensions of the biaxial tensile test on a cruciform sample [5].

Two case studies were analyzed, each employing a distinct yield criterion to describe the material's constitutive behavior: Case Study 1 utilizes the Hill'48 yield criterion, while Case Study 2 adopts the CPB'06 yield criterion. Both models assume isotropic elastic behavior, governed by Hooke's law (with Young's modulus E = 210 GPa and Poisson's ratio ν = 0.3), and isotropic hardening described by Swift law [7] under an associated flow rule.

The Hill'48 yield criterion can be written as follows (Eq. 1):

$$F(\sigma_{yy}-\sigma_{zz})^2+G(\sigma_{zz}-\sigma_{xx})^2+H(\sigma_{xx}-\sigma_{yy})^2+2L\tau_{yz}^2+2M\tau_{xz}^2+2N\tau_{xy}^2=Y^2, \quad (1)$$

where F, G, H, L, M, and N are anisotropy parameters, σ_{xx}, σ_{yy}, σ_{zz}, τ_{yz}, τ_{xz}, and τ_{xy} are the components of the Cauchy stress tensor $\boldsymbol{\sigma}$, in the material axes system of the metal sheet, and Y is the yield stress. Parameters L and M are assumed to be 1.5 (as in von Mises isotropy), and the condition $G+H = 1$ (i.e. $\sigma_{xx} = Y$) was assumed, which corresponds to the following relationships (Eq. 2):

$$F=\frac{r_0}{r_{90}(r_0+1)};\ G=\frac{1}{r_0+1};\ H=\frac{r_0}{r_0+1};\ N=\frac{1}{2}\frac{(r_0+r_{90})(2r_{45}+1)}{r_{90}(r_0+1)}, \quad (2)$$

where r_0, r_{45} and r_{90} are the Lankford coefficients obtained at 0º, 45º and 90º w.r.t. the rolling direction of the sheet, respectively.

The CPB'06 yield criterion can be written as follows (Eq. 3):

$$\left(\left|\Sigma_1\right|-k\Sigma_1\right)^a+\left(\left|\Sigma_2\right|-k\Sigma_2\right)^a+\left(\left|\Sigma_3\right|-k\Sigma_3\right)^a=Y^a, \tag{3}$$

where Σ_1, Σ_2, and Σ_3 are the principal values of the transformed deviatoric stress tensor $\mathbf{\Sigma} = \mathbf{C}\boldsymbol{\sigma}'$ where $\mathbf{C}$ is a constant fourth-order tensor containing 9 independent anisotropy parameters, given by Eq. 4:

$$\mathbf{C}=\begin{bmatrix} C_{11} & C_{12} & C_{13} & & & \\ C_{12} & C_{22} & C_{23} & & & \\ C_{13} & C_{23} & C_{33} & & & \\ & & & C_{44} & & \\ & & & & C_{55} & \\ & & & & & C_{66} \end{bmatrix}. \tag{4}$$

The Swift law describes the yield stress evolution during plastic deformation as follows (Eq. 5):

$$Y=K\left[\left(\frac{\sigma_0}{K}\right)^{1/n}+\bar{\varepsilon}^{\mathrm{p}}\right]^n, \tag{5}$$

where $\bar{\varepsilon}^{\mathrm{p}}$ is the equivalent plastic strain and σ_0, K and n are material parameters.

Dataset generation

Using the Latin Hypercube Sampling (LHS) method, a total of 9,045 simulations were generated for Case Study 1 (Hill'48), and 10,550 simulations for Case Study 2 (CPB'06). Each simulation had an average computation time of 10 seconds, utilizing a 13th Generation Intel® Core™ i9-13900 24-core processor (2.00–5.60 GHz) with 32 GB of RAM. The input space and step sizes for the material parameters to be calibrated are detailed in Table 1. Numerical simulations of the cruciform tensile test were performed while maintaining the same geometry, boundary conditions and elastic properties. In Case Study 1, 3,470 out of 9,045 simulations were selected as they exhibited no decrease in load during the simulation, meaning they did not surpass the necking point before the 20th time step. Similarly, in Case Study 2, 4,750 out of 10,550 simulations met this criterion. Then, the dataset was randomly split into two subsets: in Case Study 1, 3,000 samples were used for training and 470 for testing, while in Case Study 2, 4,000 samples were used for training and 750 for testing. Each of the training and test sets consist of two matrices: a feature matrix and a target matrix. The feature matrix has shape $n_{\text{samples}}\times n_{\text{features}}$, where n_{samples} is the total number of samples (i.e. numerical simulations) of each set (Case Study 1: n_{samples}=3,470; Case Study 2: n_{samples}=4,750) and n_{features} is the total number of features (20 timesteps×(2 forces + 3 strain components × 564 elements) = 33880 features). The target matrix has shape $n_{\text{samples}}\times n_{\text{outputs}}$, where n_{outputs} is the total number of model outputs (i.e. material parameters – Case Study 1: n_{outputs}=6; Case Study 2: n_{outputs}=9).

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Table 1 – Input space and step sizes for the material parameters under case studies 1 and 2.

	Material Parameters	Input Space	Step
Case Study 1 (Hill'48)	r_0	0.6 – 6.0	0.001
	r_{45}	0.6 – 6.0	0.001
	r_{90}	0.6 – 6.0	0.001
	K [MPa]	280 – 700	0.01
	σ_0 [MPa]	120 – 300	0.01
	n	0.100 – 0.300	0.001
Case Study 2 (CPB'06)	C_{22}	-0.5 – 2.5	0.0001
	C_{33}	-0.5 – 2.5	0.0001
	C_{12}	-1.5 – 1.5	0.0001
	C_{13}	-1.5 – 1.5	0.0001
	C_{23}	-1.5 – 1.5	0.0001
	C_{66}	-1.5 – 1.5	0.0001
	K [MPa]	280 – 700	0.01
	σ_0 [MPa]	120 – 300	0.01
	n	0.100 – 0.300	0.001

Training and testing

The training set was used for training the Extreme Gradient Boosting (XGBoost) regression algorithm; more details regarding the XGBoost algorithm can be found in [3]. The hyperparameters of the XGBoost regression algorithm were kept as default, except for the learning rate (=0.02), max_depth (=15) and n_estimators (=1000) [3]. The test set was used for evaluating the performance of the ML models in predicting the material parameters. Table 2 presents the R^2 values achieved during the training and testing phases for Case Study 1 (Hill'48) and Case Study 2 (CPB'06), highlighting the differences in model performance and generalization capabilities.

Table 2 – Comparison of R^2 values for Training and Testing in Case Study 1 (Hill'48) and Case Study 2 (CPB'06).

	Case Study 1 (Hill'48)	Case Study 2 (CPB'06)
R^2 (Train)	0.9999	0.9999
R^2 (Test)	0.9880	0.5020

The results show a clear difference in model performance between the two case studies. In Case Study 1, the high R^2 values in both training (0.9999) and testing (0.9880) indicate strong generalization, likely due to the simpler structure and lower material parameter count of the Hill'48 yield criterion. Conversely, in Case Study 2, while the training R^2 remains high (0.9999), the testing value drops significantly (0.5020), suggesting overfitting. This performance gap highlights the greater complexity of the CPB'06 yield criterion and its increased sensitivity to training data, pointing to the need for larger datasets or improved training strategies to enhance generalization. Fig. 2 and Fig. 3 provide a more detailed analysis on the performance of the ML models in predicting material parameters for the test sets of Case Study 1 (Hill'48) and Case Study 2 (CPB'06), respectively.

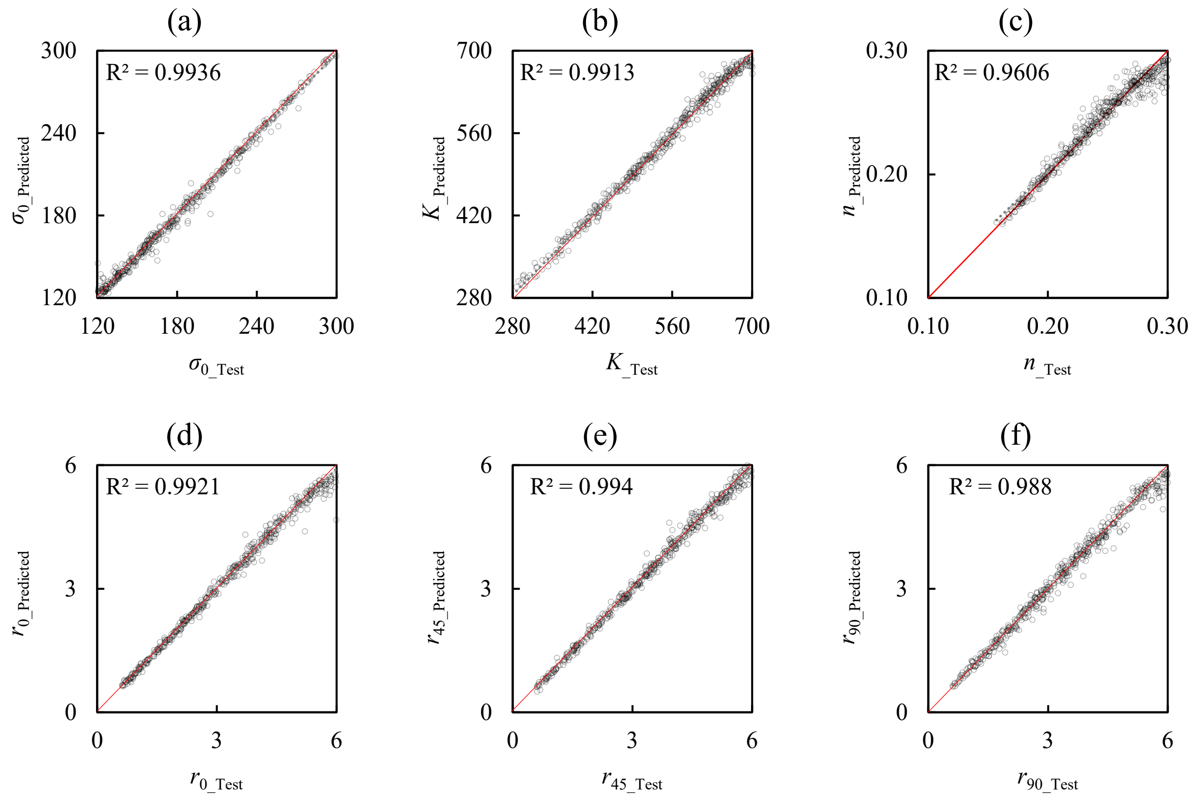
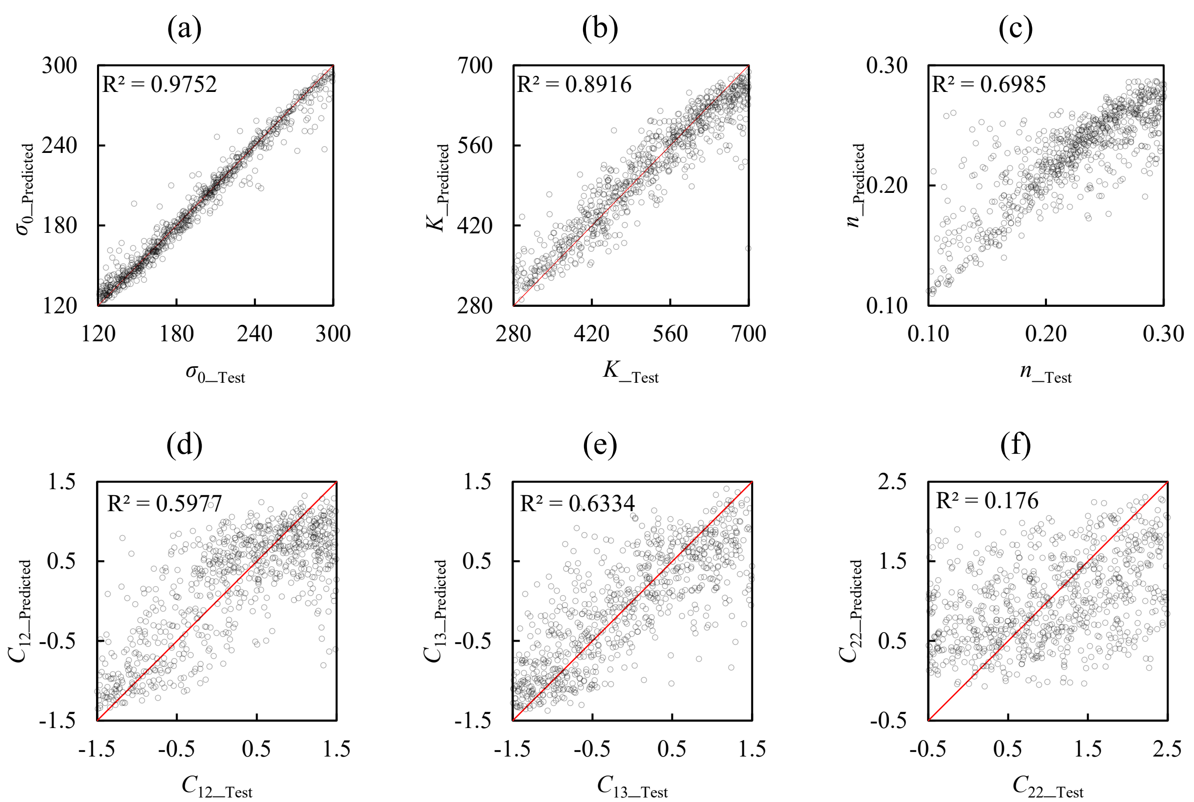


Figure 2 – Evaluation of material parameter predictions for the test set (Case Study 1): (a) σ_0, (b) K, (c) n, (d) r_0, (e) r_{45}, and (f) r_{90}.



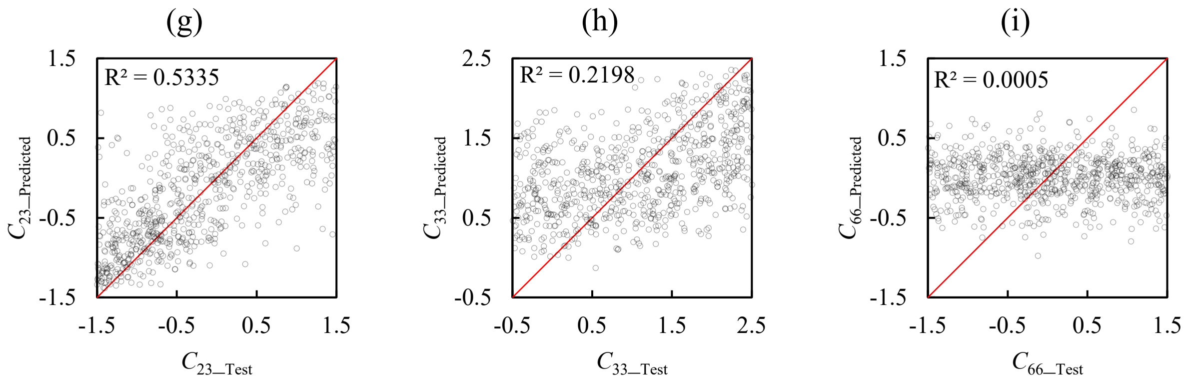


Figure 3 – Evaluation of material parameter predictions for the test set (Case Study 2): (a) σ_0; (b) K; (c) n; (d) C_{12}; (e) C_{13}, (f) C_{22}, (g) C_{23}, (h) C_{33}, and (i) C_{66}.

The Hill'48 ML model (Case Study 1) shows strong predictive performance, accurately capturing the six material parameters. In contrast, the CPB'06 ML model (Case Study 2) underperforms, with inconsistent predictions and lower R^2 values, suggesting overfitting. The model struggles to map the relationship between the input data (feature matrix) and the output data (target matrix), likely due to the criterion's inherent complexity.

Sensitivity to the training sample size

The training sets for both case studies were divided into multiple subsets to assess the performance of the machine learning models with different amounts of training data. In Case Study 1 (Hill'48), training subsets included 500, 1,000, 1,500, 2,000, and 2,500 samples, as well as the full training set of 3,000 samples. In Case Study 2 (CPB'06), subsets of 500, 1,000, 1,500, 2,000, 2,500, 3,000, and 3,500 samples were used, along with the full training set of 4,000 samples.

Fig. 4 illustrates the sensitivity analysis of the training dataset size on the R^2 metric for Case Study 1 and Case Study 2, highlighting the differing trends in model performance as the dataset size increases. A sensitivity analysis on the training dataset size revealed distinct trends in R^2 performance for both case studies. In Case Study 1, R^2 improved consistently with increasing dataset size, reflecting the model's ability to generalize effectively due to the simpler structure and lower parameter count of the Hill'48 yield criterion. Conversely, in Case Study 2, R^2 gains were slower and eventually plateaued at about $R^2 = 0.50$, suggesting that the higher parameter count and the non-linear dependencies between material parameters in the CPB'06 yield criterion pose greater challenges for model training. These results highlight the different sensitivities of the two models to dataset size, emphasizing the influence of yield criterion complexity on training effectiveness. The low R^2 for CPB'06 may stem from parameter insensitivity. Identifying and fixing weakly influential parameters or excluding them from training could improve generalization. Future work could explore this refinement.

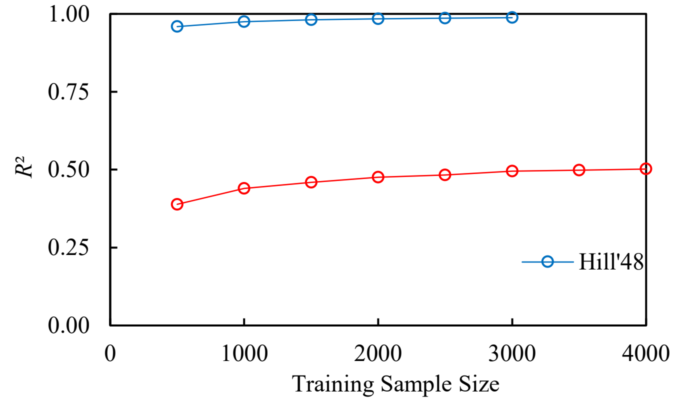


Figure 4 – Sensitivity analysis of the training sample size on the R² metric for the test set for Case Study 1 (Hill'48) and Case Study 2 (CPB'06).

Conclusions

This study evaluated the performance of XGBoost-based machine learning models in predicting material parameters for two yield criteria: Hill'48 (Case Study 1) and CPB'06 (Case Study 2), using numerical simulations of a biaxial tensile test on a cruciform sample. The Hill'48 ML model demonstrated strong predictive accuracy, with consistently high R^2 values in both training (0.9999) and testing (0.9880) phases. Its simpler structure and lower parameter count facilitated effective generalization, even with moderate dataset sizes. In contrast, the CPB'06 ML model achieved high accuracy in training ($R^2 = 0.9999$) but significantly lower performance during testing ($R^2 = 0.5020$), indicating overfitting and difficulties in capturing the non-linear parameter interactions inherent to the CPB'06 yield criterion. A sensitivity analysis on dataset size revealed that the Hill'48 ML model consistently improved with larger training sets, while the CPB'06 ML model plateaued, suggesting that dataset size alone may not fully address its training challenges. These results underscore the importance of yield criterion complexity in ML model performance and highlight the need for optimized training strategies or potentially larger, more diverse datasets when dealing with complex constitutive models like CPB'06.

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