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MACHINE LEARNING-BASED INVERSE METHOD FOR DETERMINING ELASTIC COEFFICIENTS OF UNSYMMETRIC LAMINATES

INVERZNA METODA ZASNOVANA NA MAŠINSKOM UČENJU ZA ODREĐIVANJE KOEFICIJENATA ELASTIČNOSTI NESIMETRIČNIH LAMINATA

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Keywords
- unsymmetric laminates
- equivalent shear modulus
- inverse design
- machine learning
- LightGBM

Abstract

Determination of equivalent elastic coefficients in composite laminates is a fundamental problem in structural mechanics and materials engineering. This task becomes particularly challenging for unsymmetric laminates, where coupling effects between membrane, bending, and shear responses render analytical characterisation difficult and computationally expensive. In this work, a machine learning-based inverse methodology is proposed for determining the equivalent shear modulus of unsymmetric composite laminates. A high-fidelity finite element implementation of the ASTM V-notched shear test is used to generate a comprehensive dataset covering a wide range of unsymmetric stacking sequences. A Light Gradient Boosting Machine (LightGBM) model is trained as a nonlinear surrogate to map laminate design variables to the corresponding equivalent shear modulus. The trained model is subsequently employed in an inverse design framework to identify laminate stacking sequences that achieve prescribed target values of shear modulus. The proposed approach significantly reduces computational cost compared to conventional trial-and-error finite element analysis and provides new insight into the relationship between laminate architecture and effective shear behaviour.

Ključne reči
- asimetrični laminati
- ekvivalentni modul smicanja
- inverzno projektovanje
- mašinsko učenje
- LightGBM

Izvod

Određivanje ekvivalentnih koeficijenata elastičnosti kompozitnih laminata predstavlja jedan od problema strukturalne analize konstrukcija. Ovaj problem postaje posebno izazovan kod asimetričnih laminata, gde efekti sprezanja između membranskog, savojnog i smičućeg odziva otežavaju analitičku karakterizaciju i čine je računski zahtevnom. U ovom radu predložena je inverzna metodologija zasnovana na mašinskom učenju za određivanje ekvivalentnog modula smicanja asimetričnih kompozitnih laminata. Implementacija metode konačnih elemenata testa smicanja ASTM V-zareza korišćena je za generisanje sveobuhvatnog skupa podataka koji pokriva širok spektar asimetričnih slaganja slojeva. Model Light Gradient Boosting Machine (LightGBM) obučen je kao nelinearni model za mapiranje nesimetričnih laminata na odgovarajući ekvivalentni modul smicanja. Obučeni model je primenjen u inverznom projektnom okviru radi identifikacije redosleda slaganja laminata koji postižu ciljne vrednosti modula smicanja. Predloženi pristup značajno smanjuje procesorsko vreme u poređenju sa konvencionalnom analizom metodom pokušaja i grešaka metodom konačnih elemenata i pruža nove uvide u vezu između arhitekture laminata i efektivnog smičućeg ponašanja.

INTRODUCTION

Fiber-reinforced composite laminates have emerged as essential materials in weight-critical engineering applications, from primary aerospace structures to automotive and civil infrastructure, due to their superior specific strength and stiffness and the ability to tailor mechanical response through controlled ply orientations and stacking sequences /1-4/. Among the laminate macroscopic elastic properties, the equivalent in-plane shear modulus is of particular significance, as it governs in-plane load transfer, transverse shear stiffness, torsional rigidity of thin-walled members, and coupled deformation modes, which are critical for the performance of thin-walled structures and aeroelastic stability of lifting surfaces, /2/.

For symmetric laminates, where ply orientations are mirrored about the mid-plane, the coupling matrix vanishes, and Classical Lamination Theory provides closed-form expressions for equivalent elastic coefficients, including the shear modulus /1-3/. This analytical tractability, along with predictable cure-induced behaviour and minimal thermal warpage, has made symmetric laminates standard in primary aerospace components such as wing skins, fuselage shells, and bulkheads, /4/.

Unsymmetric laminates lack mid-plane mirror symmetry, producing a non-zero coupling matrix and inducing extension-bending, extension-twist, and bending-twist coupling /5, 6/. These nonlinear interactions make the effective elastic properties highly configuration-dependent, precluding simple analytical expressions and necessitating high-fidelity finite element simulations, /2/. Residual stresses during curing further complicate the structural response, often inducing warpage that must be accounted for in manufacturing and assembly /7-9/. Nevertheless, unsymmetric laminates offer significant advantages when their coupling effects are intentionally exploited. They enable passive aeroelastic tailoring /10/, allowing wings to reduce tip deflection under load, modify angle of attack to alleviate gust loads, and delay flutter onset through optimised stiffness distribution, /11/. Unsymmetric laminates also allow for weight reduction by integrating multiple structural functions within a single configuration, reducing the number of required plies without compromising performance. Furthermore, controlled residual stresses from unsymmetric stacking can produce predictable out-of-plane deformation, a principle exploited in tape-spring booms for satellites, /12, 13/, morphing leading or trailing edges, and self-deploying airbrakes and fairings /13/. Documented aerospace applications include bending-twist coupled rotor blades /5/, passive flutter suppression in composite wings /11/, deployable composite booms such as the Roll-Out Solar Array /14/, and unavoidable unsymmetric configurations in field repair patches.

The adoption of unsymmetric laminates is challenged by manufacturing distortions, as the non-zero coupling matrix generates residual stresses during curing that can cause warping and requires careful tooling and process control /8, 15/. Capturing coupled membrane, bending, and shear responses necessitates advanced finite element modelling and experimental validation, /2/. Moreover, the non-standard behaviour of unsymmetric laminates complicates compliance with aerospace certification requirements, including FAA and EASA regulations /16, 17/. Despite these challenges, the unique functional advantages of unsymmetric laminates make them highly attractive for advanced aerospace applications, motivating the need for efficient design strategies.

The computational expense of exploring unsymmetric laminate design spaces is substantial, as the nonlinear mapping between ply angles, stacking sequence, and effective shear modulus requires extensive finite element simulation or experimental evaluation to identify configurations meeting target mechanical requirements, /2, 11/. Conventional trial-and-error approaches are prohibitively expensive in industrial design cycles, highlighting the need for efficient surrogate models capable of accurately predicting shear modulus across high-dimensional, discontinuous design spaces /18-20/.

In this context, the Light Gradient Boosting Machine presents an ideal framework, /21/. As an ensemble-based gradient boosting algorithm, it constructs highly accurate predictive models by sequentially fitting decision trees to capture nonlinear and discontinuous relationships between laminate design variables, such as ply angles, layer thicknesses, and stacking order, and the resulting equivalent shear modulus /18, 21/. Its inherent handling of high-dimensional input spaces, robustness to outliers, and computational efficiency make it particularly suitable for composite laminate design problems, /20, 21/.

Building on the predictive capability of LightGBM, this work integrates an inverse design algorithm that leverages the trained surrogate model to identify laminate stacking sequences achieving prescribed target shear modulus values /19, 22, 23/. The inverse algorithm efficiently searches the design space using randomised and heuristic strategies, circumventing the need for exhaustive finite element evaluation, /22/. This approach enables rapid exploration of unsymmetric laminate architectures, providing actionable insights into the effects of asymmetry on shear performance and significantly reducing computational cost relative to traditional design workflows.

Building on this motivation, the subsequent methodology implements a three-step framework for predicting and inversely designing equivalent shear modulus in unsymmetric laminates. First, high-fidelity finite element simulations are conducted across a broad range of unsymmetric stacking sequences to generate a comprehensive dataset linking ply angles and stacking order to the resulting shear modulus /2, 11/. Second, a LightGBM surrogate model is trained on this dataset to capture the complex, nonlinear mapping from laminate architecture to shear response, leveraging its gradient boosting tree ensemble to efficiently handle discontinuities and high-dimensional input spaces /18, 20, 21/. Finally, the trained surrogate model is integrated with an inverse design algorithm that systematically searches for stacking sequences achieving prescribed target shear modulus values /19, 22, 23/. By decoupling the prediction of shear modulus from expensive finite element simulations, this approach enables rapid exploration of the laminate design space, allowing for efficient identification of feasible unsymmetric architectures while quantifying the influence of ply asymmetry on shear behaviour, /20/.

METHODS AND MATERIALS

The ASTM D7078 V-notched rail shear test is a standardised experimental procedure for determining the in-plane shear response of composite laminates. The test geometry and loading configuration are specifically designed to promote a dominant shear stress state within the gauge section of the specimen while suppressing global bending modes.

For symmetric laminates, interpretation of measured force-displacement response is relatively straightforward, as the deformation is largely governed by uniform in-plane shear.

For unsymmetric laminates, however, elastic coupling between membrane, bending, and twisting deformation modes may occur, leading to non-uniform stress and strain fields throughout the specimen thickness and along the gauge region. These coupling effects complicate the interpretation of local strain measurements and invalidate simplified kinematic assumptions commonly used for symmetric configurations.

To address these challenges, a high-fidelity finite element framework is employed to numerically simulate the V-notched rail shear test under controlled boundary conditions. The FEA model and set-up are presented in Fig. 1.

Each laminate configuration is modelled explicitly at the ply level, incorporating orthotropic material behaviour, detailed stacking sequence definitions, and boundary conditions consistent with the ASTM D7078 standard. The finite element formulation ensures equilibrium and compatibility while fully accounting for anisotropy and coupling effects inherent to unsymmetric laminates.

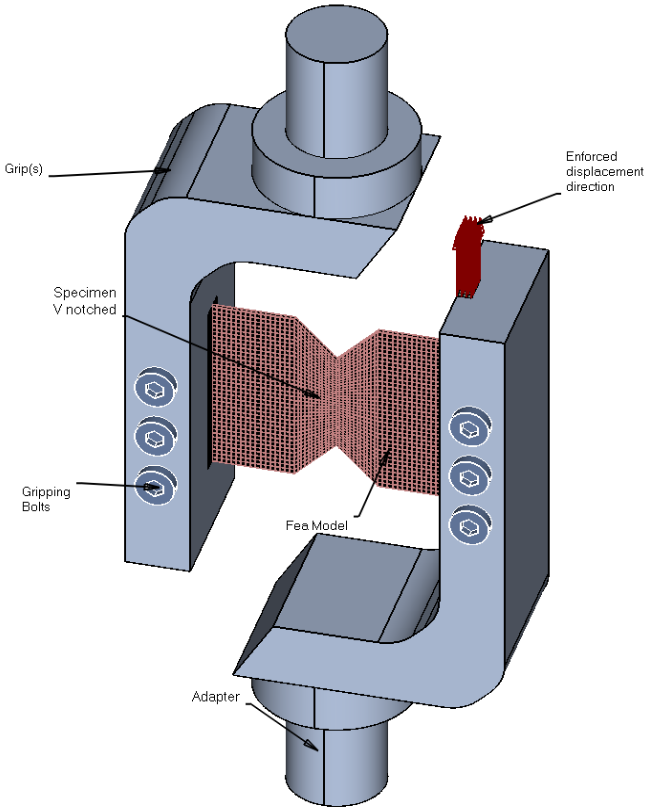

Figure 1. FEA model and set-up.

Figure 2 illustrates the finite element model of the V-notched specimen, including the imposed shear deformation and representative stress or strain field contours obtained from the simulation.

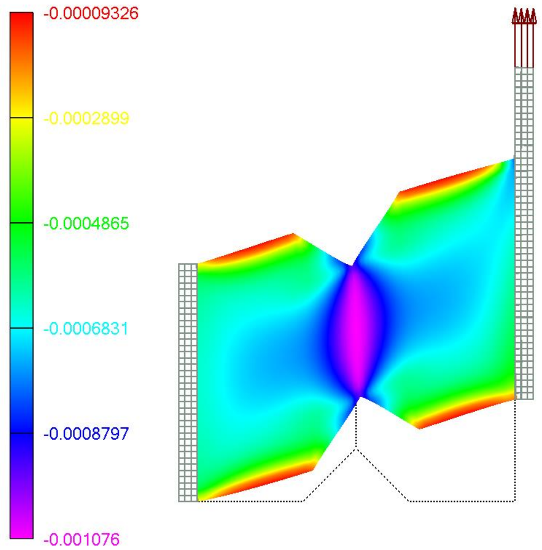

Figure 2. Shear deformation of a V-notch sample.

Rather than relying on local strain measurements or simplified kinematic assumptions, an energy-based interpretation is adopted to extract an equivalent shear modulus directly from global reaction forces and imposed displacements. This approach is particularly well suited for unsymmetric laminates, as it remains valid in the presence of non-uniform stress and strain fields.

For a linearly elastic body subjected predominantly to shear deformation, the shear contribution to the internal strain energy is expressed as

$$U_{shear} = \frac{1}{2}\int_V \tau(x,y,z)\gamma(x,y,z)dV \,, \tag{1}$$

where: τ and γ denote local shear stress and shear strain fields, respectively; and V is total specimen volume. This formulation explicitly accounts for non-uniform stress and strain distributions arising from elastic coupling effects in unsymmetric laminates.

Within the finite element framework, these stress and strain fields satisfy equilibrium and compatibility, ensuring that the computed strain energy is energetically consistent.

In the limiting case of approximately uniform shear fields, the expression reduces to

$$U_{shear} = \frac{1}{2}\tau\gamma V \,, \tag{2}$$

which is useful for interpretation but not required for the general formulation.

The external work performed by the applied shear force during a prescribed displacement is given by:

$$U_{ext} = \int_0^{\Delta} F_y d\delta \,. \tag{3}$$

Assuming linear elastic behaviour and monotonic loading, the force-displacement response is linear, yielding:

$$U_{ext} = \frac{1}{2}F_y\Delta \,. \tag{4}$$

According to the principle of virtual work, the internal strain energy must equal the external work,

$$U_{shear} = U_{ext} \,. \tag{5}$$

Substitution leads to

$$\frac{1}{2}\int_V \tau(x,y,z)\gamma(x,y,z)dV = \frac{1}{2}F_y\Delta \,. \tag{6}$$

For uniform shear fields, this relation reduces to

$$\frac{1}{2}\tau\gamma V = \frac{1}{2}F_y\Delta \,. \tag{7}$$

Introducing the effective shear stress, specimen volume, and macroscopic shear strain, the equivalent shear strain is defined as:

$$\gamma_{eq} = \frac{\Delta}{L_{eff}} \,. \tag{8}$$

The equivalent shear modulus is defined through the macroscopic constitutive relation

$$G_{eq} = \frac{\tau_{eq}}{\gamma_{eq}} \,, \tag{9}$$

where equivalent shear stress is obtained from the global reaction force as

$$\tau_{eq} = \frac{F_y}{wt} \,. \tag{10}$$

Combining the above expressions yields,

$$G_{eq} = \frac{F_y}{wt}\frac{L_{eq}}{\Delta} \,. \tag{11}$$

This definition is entirely energy-consistent and remains valid for both symmetric and unsymmetric laminates. All coupling effects and stress non-uniformities are implicitly captured through the global force-displacement response obtained from FEA. In previous equations G_{eq} represents equivalent in-plane shear modulus obtained from energy equivalence, F_y is global reaction shear force obtained from the rail supports in the loading direction, w is width of the shear specimen measured between the notches, t is thickness of composite specimen, L_{eff} is effective shear length between the notches over which deformation is assumed, and Δ is imposed relative shear displacement applied during the test or FEA simulation.

In the present analysis, the commercial finite element solver NASTRAN® is employed to simulate the ASTM D7078 V-notched rail shear test.

The composite specimen is modelled using laminate shell elements of the LAMINATE formulation, implemented through four-node quadrilateral shell elements with layered composite capability. These elements are based on classical lamination theory and are capable of accurately representing membrane, bending, and membrane-bending coupling behaviour arising in unsymmetric laminates.

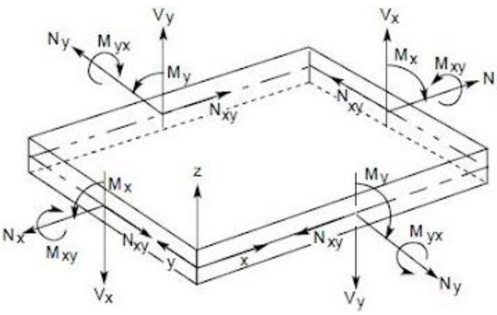

Figure 3. NASTRAN® laminate element forces and moments.

The laminate definition is introduced through the PCOMP bulk data entry, which allows multiple composite plies to be associated with a single shell element. Each ply is characterised by its thickness, material identification, and fibre orientation angle.

Through this formulation, stiffness matrices A, B, and D are implicitly constructed at the element level, enabling the capture of elastic coupling effects without the need for three-dimensional solid modelling.

This approach provides an efficient and physically consistent representation of laminated composite behaviour, particularly suitable for large-scale parametric studies. An illustrative example of a PCOMP entry used in the present study is given in Table 1.

Table 1. NASTRAN PCOMP entry for composite laminate.

PCOMP	1001	1	0.0	YES
+	1	0.125	45.0	YES
+	1	0.125	-45.0	YES
+	1	0.125	30.0	YES

In this example, the PCOMP entry defines a four-ply laminate associated with a shell property identification number.

Each continuation line corresponds to a single ply within the laminate stack. The material identification number refers to an orthotropic composite material defined separately using MAT8 entries. The ply thickness specifies the physical thickness of each lamina, while the orientation angle defines the fibre direction relative to the element reference coordinate system. The final flag indicates whether the ply contributes to the laminate stiffness and mass.

Since the primary objective of the present work is the generation of a large and diverse dataset suitable for machine learning applications, a fully automated data generation strategy is adopted. A dedicated preprocessing routine is developed to programmatically modify the NASTRAN input file prior to each solver run.

This routine directly targets the PCOMP entry and systematically updates the ply orientation angles before each analysis. For every simulation, new ply angles are generated by random sampling within the range of -90 to +90 degrees, while maintaining fixed ply thicknesses and material properties.

The complete workflow, including modification of the PCOMP entries, execution of NASTRAN solver, and post-processing of reaction forces and imposed displacements, is fully automated. This strategy enables the efficient generation of a substantial number of energetically consistent data points, each corresponding to a unique unsymmetric laminate configuration.

The resulting dataset forms a reliable foundation for subsequent machine learning training and inverse analysis, while preserving direct physical linkage to the underlying finite element simulations.

Each laminate configuration's equivalent shear modulus derives from FEA data and the energy formulation in Eq.(11).

Although the laminate formulation is based on classical lamination theory, the equivalent shear modulus is not extracted from laminate constitutive relations but is defined exclusively through an energy-equivalence principle at the structural level, ensuring validity for unsymmetric laminates with strong elastic coupling.

The dataset employed in the present study is constructed to support the development of a robust machine learning surrogate model for predicting the equivalent in-plane shear modulus of composite laminates, with particular emphasis on unsymmetric stacking sequences. Given the statistical nature of regression-based machine learning methods, careful attention is paid to dataset representativeness, balance, and coverage of the laminate design space.

It should be emphasised that the employed machine learning framework is fundamentally statistical in nature.

Consequently, when the training dataset is generated via finite element simulations combined with randomised fibre orientation sampling, there is no guarantee that symmetric laminate configurations will naturally occur with sufficient frequency.

Although the primary objective of the present study is the characterisation of unsymmetric laminates, from a statistical learning perspective, it is beneficial to explicitly include symmetric layups within the dataset in order to improve the overall representativeness of the design space.

To this end, several hundred symmetric laminate configurations are deliberately generated and incorporated into the dataset. In order to reduce computational cost, these configurations are evaluated using Classical Lamination Theory (CLT) rather than full FEA.

For each symmetric laminate, the ABD stiffness matrix is computed, and the equivalent in-plane shear modulus is evaluated using an energy-equivalence formulation, expressed as

$$G_{xy}^{eq} = \frac{12}{t^3} D_{66}^{*}, \qquad (12)$$

where: t is total laminate thickness; and D_{66}^{*} is the component of the inverse ABD matrix.

This hybrid data generation strategy ensures adequate statistical coverage of both symmetric and unsymmetric laminate behaviours while maintaining computational efficiency.

It is well known that most regression-based machine learning algorithms exhibit limited extrapolation capability outside the domain spanned by training data. As a result, predictions near or beyond the boundaries of the design space may become unreliable if such regions are insufficiently represented during training.

To mitigate this limitation, additional ‘hard’ boundary points are computed and explicitly included in the dataset, corresponding to extreme but physically admissible fibre orientation angles within the laminate design space. These boundary samples serve to anchor the regression model at the limits of feasible layup configurations and reduce uncontrolled extrapolation effects. By explicitly enforcing coverage of the design space boundaries, the prediction reliability near extreme fibre orientations is significantly improved.

This strategy contributes not only to more stable forward predictions of the equivalent shear modulus, but also to enhanced robustness of inverse laminate design procedures, where target stiffness values may correspond to configurations located near the edges of the admissible domain.

Prior to training the regression models, the combined dataset-comprising FEA-based unsymmetric laminates and CLT-based symmetric laminates - was randomly shuffled. This preprocessing step is essential to prevent unintended ordering effects during training, which may otherwise bias the learning process toward specific laminate families.

Dataset shuffling promotes faster convergence of the regression algorithm and contributes to improved generalisation performance, as reflected by higher and more stable values of the coefficient of determination R^2 across training and validation sets. Following the generation of the combined dataset, consisting of finite element-based unsymmetric laminate data and CLT-based symmetric laminate data, a random shuffling procedure is applied prior to machine learning model training. This step is essential to eliminate ordering bias associated with sequential data generation and to ensure statistically consistent learning behaviour.

In the present workflow, finite element simulations and CLT-based computations are performed in separate batches and subsequently merged into a single dataset. Without shuffling, this could result in contiguous blocks of data with similar laminate characteristics or stiffness levels being presented consecutively to the learning algorithm. Such ordering effects can bias gradient-based optimisation, slow convergence, and lead to optimistic or misleading estimates of model accuracy.

Random shuffling ensures that laminate configurations with different stacking symmetries, coupling characteristics, and equivalent shear modulus values are uniformly distributed throughout the training process. As a result, each training batch contains a statistically representative mixture of data samples, which promotes smoother optimisation trajectories and accelerates convergence during training.

From a performance perspective, shuffling contributes directly to improved and more stable estimates of the coefficient of determination R^2, as the validation sets are no longer dominated by narrowly clustered stiffness regimes. This leads to a more reliable assessment of generalisation capability and reduces variance in performance metrics across cross-validation folds.

From an inverse design standpoint, shuffling the dataset further enhances robustness by ensuring that similar output values of the equivalent shear modulus correspond to diverse and decorrelated laminate configurations within the training process. This reduces the risk of the regression model overfitting to local patterns and improves its reliability when used in inverse searches for laminate designs matching a prescribed target shear modulus.

Furthermore, dataset shuffling enhances the robustness of the inverse design process. Since inverse searches rely on the global smoothness and consistency of the learned forward mapping between laminate parameters and equivalent shear modulus, a well-mixed training dataset reduces the risk of localised bias in the surrogate model. This improves the reliability of inverse predictions, particularly when exploring laminate configurations near the boundaries between symmetric and unsymmetric regimes.

Prior to training and evaluating regression models, a dedicated data preprocessing stage is applied to ensure the physical consistency and numerical reliability of the finite element generated dataset. Although the dataset is synthetically generated using high-fidelity finite element simulations, unsymmetric laminate configurations are known to exhibit strong elastic coupling effects, which may occasionally lead to non-physical responses or numerical instabilities for extreme stacking sequences. Such effects can manifest as outlier values in the equivalent shear modulus or inconsistent force-displacement responses, potentially biasing the machine learning model if left unaddressed.

To mitigate this risk, an anomaly detection procedure based on Principal Component Analysis (PCA) is employed as a data validation and filtering step. The PCA is a linear dimensionality reduction technique that projects high-dimensional data onto a lower-dimensional orthogonal subspace defined by directions of maximum variance.

In the present context, the input feature space consists of laminate design variables, including fibre volume fraction and ply orientation angles, while the output corresponds to the equivalent shear modulus obtained from energy-equivalent finite element analysis.

The PCA model is trained using the standardised dataset, and a reduced set of principal components is retained such that the majority of the total variance is preserved. Each data point is then projected onto the retained subspace and reconstructed back into the original feature space.

The reconstruction error, defined as the norm of the difference between the original and reconstructed data, is used as an anomaly score. Data points exhibiting reconstruction errors exceeding a prescribed threshold are classified as anomalous and excluded from subsequent analysis.

This approach enables the identification of data samples that deviate significantly from the dominant statistical structure of the dataset, which may arise from numerical convergence issues, atypical deformation modes, or extreme coupling behaviour in unsymmetric laminates. Importantly, the PCA-based anomaly detection is used solely as a preprocessing and quality assurance tool and does not impose any assumptions on the underlying constitutive behaviour.

The PCA-based anomaly detection procedure applied to dataset created is briefly outlined mathematically in the following text. Standardised dataset is denoted, in mathematical form as:

$$\mathbf{X} \in \mathbb{R}^{N\times d}, \quad (13)$$

where: N is the number of laminate configurations; and d is the number of input and output features.

The covariance matrix of the dataset is defined as

$$\mathbf{C} = \frac{1}{N-1}\mathbf{X}^T\mathbf{X}. \quad (14)$$

Principal components are obtained by solving the eigenvalue problem

$$\mathbf{C}\mathbf{v}_k = \lambda_k \mathbf{v}_k, \quad (15)$$

where: λ_k and $\mathbf{v}_k$ denote the eigenvalues and corresponding eigenvectors, respectively.

The eigenvectors are ordered by decreasing eigenvalue magnitude, and the first r components are retained to form the projection matrix

$$\mathbf{V}_r = [\mathbf{v}_1, \ldots, \mathbf{v}_r]. \quad (16)$$

Each data point $\mathbf{x}_i$ is projected onto reduced subspace as

$$\mathbf{z}_i = \mathbf{V}_r^T \mathbf{x}_i, \quad (17)$$

and reconstructed back into the original space as

$$\hat{\mathbf{x}}_i = \mathbf{V}_r \mathbf{z}_i. \quad (18)$$

The anomaly score is defined using the reconstruction error

$$e_i = \left\|\mathbf{x}_i - \hat{\mathbf{x}}_i\right\|^2, \quad (19)$$

which quantifies the deviation of a sample from the dominant statistical structure of the dataset. Samples with reconstruction errors exceeding a prescribed threshold are classified as anomalous and removed prior to regression model training.

After the removal of anomalous samples, the resulting dataset exhibits improved statistical consistency and physical plausibility, providing a robust foundation for regression model training and algorithm comparison. The cleaned dataset is subsequently used for evaluating multiple regression algorithms and for training the final LightGBM surrogate model employed in both forward prediction and inverse laminate design.

MACHINE LEARNING FRAMEWORK

The determination of the equivalent in-plane shear modulus from laminate design variables constitutes a nonlinear regression problem characterised by strong feature interactions and pronounced sensitivity to stacking sequence variations. This complexity is particularly evident for unsymmetric laminates, where elastic coupling effects lead to highly non-uniform stress and strain fields that cannot be captured through simplified analytical models.

In the present work, the equivalent shear modulus G_{eq} obtained from energy-equivalent finite element simulations of the ASTM D7078 V-notched rail shear test serves as the target variable for supervised learning. The input feature vector consists exclusively of physically meaningful laminate design parameters, such as ply orientation angles and laminate configuration descriptors, ensuring that the learning problem remains directly grounded in structural mechanics.

Given the computational cost associated with generating high-fidelity finite element data, the available dataset is of moderate size. Consequently, the selection of an appropriate machine learning algorithm must balance predictive accuracy, robustness to nonlinear feature interactions, and computational efficiency. Since the objective is the prediction of continuous-valued mechanical properties, the problem is naturally formulated as a regression task.

Several regression algorithms commonly employed in structural and materials modelling are evaluated to identify the most suitable surrogate modelling approach for the present problem. The candidate algorithms include Stochastic Dual Coordinate Ascent (SDCA) regression, Fast Forest regression, Fast Tree regression, and Light Gradient Boosting Machine (LightGBM).

Each algorithm is trained using the same finite element-generated dataset and identical input feature sets. Model performance is assessed using the coefficient of determination R^2 as the primary accuracy metric, while computational efficiency is evaluated based on training time and convergence behaviour. Particular emphasis is placed on achieving the highest possible predictive accuracy within the shortest training time, reflecting practical engineering requirements for rapid surrogate model development, Table 2.

Table 2. Algorithm selection.

Algorithm	R^2 [-]	Training time [s]
SDCA Regression	0.11	356
Fast Tree Regression	0.35	407
Fast Forest Regression	0.44	428
LightGBM	0.65	370

Based on this comparative evaluation, LightGBM is selected as the surrogate modelling framework for the present study. Its favourable balance between accuracy and computational efficiency makes it particularly well suited for regression problems arising in composite laminate characterisation, where data generation is expensive and strong nonlinear coupling effects dominate the response.

The accurate prediction of equivalent shear modulus in composite laminates presents a significant challenge, particularly for unsymmetric stacking sequences, where small changes in ply orientation can induce substantial variations in global shear response. High-fidelity finite element analysis is therefore used to generate a comprehensive dataset spanning a wide range of unsymmetric laminate configurations. For each configuration, the equivalent shear modulus is computed using the energy-equivalence formulation described previously, ensuring that all training labels are energetically consistent and physically admissible.

LightGBM is an efficient implementation of gradient boosting decision trees, constructing an additive predictive model of the form

$$F_M(\mathbf{x}) = \sum_{m=1}^{M} \eta h_m(\mathbf{x}), \tag{20}$$

where: $\mathbf{x}$ is vector of laminate design variables; $h_m(\mathbf{x})$ is the weak learner at boosting iteration m; η is learning rate; and M is total number of boosting rounds.

At each iteration, the model minimises a differentiable loss function $L(y, \hat{y})$ by fitting the negative gradient of the loss with respect to the current prediction,

$$r_{im} = -\left.\frac{\partial L(y_i, \hat{y}_i)}{\partial \hat{y}_i}\right|_{\hat{y}_i = F_{m-1}(\mathbf{x}_i)}. \tag{21}$$

LightGBM employs a leaf-wise tree growth strategy, in which the leaf that produces the maximum reduction in the objective function is selected for splitting. For a given leaf, aggregated gradient and Hessian statistics are computed as

$$G = \sum_{i \in leaf} g_i, \quad H = \sum_{i \in leaf} h_i, \tag{22}$$

where: g_i and h_i denote the first and second derivatives of the loss function with respect to the model prediction.

The optimal leaf weight minimising the regularised objective function

$$\mathcal{L}(w) = \sum_{i \in leaf} \left(g_i w + \frac{1}{2} h_i w^2 \right) + \frac{\lambda}{2} w^2, \tag{23}$$

is obtained in closed form as

$$w^* = -\frac{G}{H + \lambda}, \tag{24}$$

where: λ is the regularisation parameter.

The gain associated with splitting a parent leaf into left and right child leaves is given by

$$\Delta\mathcal{L} = \frac{1}{2}\left(\frac{G_L^2}{H_L + \lambda} + \frac{G_R^2}{H_R + \lambda} - \frac{(G_L + G_R)^2}{H_L + H_R + \lambda} \right). \tag{25}$$

Once trained, the LightGBM model provides a fast and accurate forward predictor of the equivalent shear modulus directly from laminate design variables. More importantly, the surrogate model enables an inverse design formulation, in which laminate configurations are identified to match prescribed target shear properties. The inverse problem is expressed as

$$\min_{\boldsymbol{\theta} \in \Omega} \left| F_M(\boldsymbol{\theta}) - G_{eq}^{target} \right|, \tag{26}$$

where: $\boldsymbol{\theta}$ is the laminate stacking sequence; and Ω represents admissible design constraints, including allowable ply angles and laminate configuration restrictions.

Although LightGBM provides strong default performance, its predictive accuracy and generalisation capability depend on appropriate selection of hyperparameters. In the present study, hyperparameter tuning is performed with the objective of maximising prediction accuracy while maintaining short training times, consistent with the practical requirement of rapid surrogate model construction.

Primary hyperparameters considered include the number of boosting iterations, learning rate, maximum tree depth, number of leaves, and regularisation parameters. The learning rate controls the contribution of each individual tree to the final model, with smaller values improving generalisation at the cost of increased training iterations. The maximal tree depth and number of leaves govern model complexity and directly influence the ability of the algorithm to capture nonlinear interactions between ply orientations.

Hyperparameter tuning is conducted using a validation-based approach, in which the dataset is split into training and validation subsets. The coefficient of determination is used as the primary metric for model evaluation. Emphasis is placed on avoiding overfitting, particularly due to the moderate dataset size and the strong nonlinear sensitivity of equivalent shear modulus to laminate configuration.

The final selected hyperparameter set achieves stable convergence, high predictive accuracy, and consistent performance across different random train-validation splits. Once trained, the LightGBM model is fixed and used for all subsequent forward predictions and inverse design studies.

CASE STUDY

To demonstrate the efficacy of proposed machine learning-based inverse method, we apply it to the aeroelastic tailoring of a composite UAV wing. The design challenge involves determining laminate elastic coefficients that simultaneously satisfy target divergence and aileron reversal speeds, a multi-objective inverse problem that is computationally expensive using traditional iterative approaches /24/.

The UAV wing features a 3.5 m span with a single-cell box beam construction (enclosed area A_m = 0.015 m^2, four-panel configuration). The aileron occupies 50 % of the semi-span with 25 % chord ratio. Key geometric, aerodynamic, and reference parameters used in the divergence calculation are summarised in Table 3.

Table 3. UAV Wing data.

Symbol	Value	Unit	Description
B	3.5	m	total wingspan
$\bar{c}$	0.35	m	mean aerodynamic chord
S	1.225	m^2	wing reference area
A_m	0.015	m^2	enclosed wing box area
J	1.08e-05	m^4	torsional constant
e	0.035	m	elastic-axis offset from aerodynamic centre
ρ	1.225	kg/m^3	air density (ISA sea level)
$dC_L/d\alpha$	5.5	rad^{-1}	lift-curve slope
V_D (target)	190	m/s	target divergence speed (near-transonic)
V_R (target)	175	m/s	target aileron reversal speed (near-transonic)

The proposed inverse method operates as follows.

Using the analytical inverse formulations derived in this work, the target divergence and reversal speeds are converted to required equivalent shear modulus values.

The required equivalent shear modulus associated with torsional divergence is obtained from the inverse divergence relation

$$G_{eq,D}^{req} = \frac{\rho\left(\dfrac{dC_L}{d\alpha}\right)Sel^2}{2J}(V_D^{target})^2 \,. \qquad (27)$$

Substituting values from Table 3 yields $G_{eq,D}$ = 8.8 GPa, whereas the aileron reversal required equivalent shear modulus is expressed as:

$$G_{eq,R}^{req} = \frac{(V_R^{target})^2 \rho \dfrac{dC_z}{d\alpha}\dfrac{\partial C_{mac}}{\partial \beta} S\bar{c}}{2J\dfrac{\partial C_z}{\partial \beta}} \,, \qquad (28)$$

yielding required aileron reversal constraint $G_{eq,R}$ = 1.7 GPa. The divergence constraint governs (significantly more stringent), establishing G_{eq} = 8.8 GPa as the design target.

LightGBM surrogate is trained on a dataset generated from finite-element simulations of V-rail shear tests for unsymmetric and symmetric laminates. The dataset contains ply configurations and associated equivalent shear modulus G_{eq} obtained from FEA. The surrogate learns the forward mapping,

$$\boldsymbol{\theta} \rightarrow G_{eq} \qquad (29)$$

with $R^2 > 0.95$ validation accuracy, enabling millisecond predictions of G_{eq} for new laminates.

Rather than iteratively searching for laminates, the inverse algorithm directly predicts candidate laminates using the surrogate gradient information. The optimisation minimizes:

$$\mathcal{L}(\boldsymbol{\theta}) = \left| f_{surrogate}(\boldsymbol{\theta}) - G_{eq}^{critical} \right| + \lambda_1 \left| V_D^{pred} - V_D^{target} \right| + \\ + \lambda_2 \left| V_R^{pred} - V_R^{target} \right| . \qquad (30)$$

Here, V^{pred} are obtained from analytical divergence and reversal equations using the surrogate-predicted G_{eq}.

The inverse algorithm converges to the following best-match laminates for AS4/epoxy, Table 4.

Table 4. Best-match laminates from inverse algorithm.

Layup type	Volume fraction	Ply angles [deg]	Predicted G_{eq} [GPa]
Asymmetric	0.491	-36, -25,-87, 3,-5	8.8
Symmetric	0.428	55, 51, 89, 51, 55	8.801
Industrial	0.523	0, -30, 0, -30, -90	8.8
Symm+Ind	0.404	30, 90, 90, 90, 30	8.82

Divergence is the active constraint, requiring significantly higher stiffness than reversal. The ML optimiser prioritises the governing physics accordingly.

The algorithm identifies that unsymmetric configurations provide the required compliance while maintaining structural integrity designs impractical to discover via manual iteration.

Forward analysis would require evaluating > 10^4 laminates to bracket the target G_{eq}. The inverse method computes the required modulus directly and identifies matching candidates in < 50 surrogate evaluations.

This case study validates that the machine learning-based inverse method enables rapid, physics-informed determination of laminate elastic coefficients for multi-constraint aeroelastic problems. By embedding analytical inverse formulations within a surrogate-based optimisation framework, the approach eliminates iterative trial-and-error, reduces computation time by three orders of magnitude, and identifies non-intuitive unsymmetric designs that satisfy stringent aeroelastic requirements.

RESULTS AND DISCUSSION

The trained LightGBM model demonstrates excellent agreement with finite element-derived equivalent shear modulus values across a wide range of unsymmetric laminate configurations. Figure references to predicted versus FEA-computed values may be included here to visually demonstrate the quality of fit.

Quantitatively, the model achieves a high coefficient of determination, indicating that dominant nonlinear relationships between ply orientations and equivalent shear response are successfully captured. This result is particularly significant given that unsymmetric laminates exhibit strong membrane-bending coupling which complicates conventional analytical estimation of shear properties.

The predictive accuracy achieved using a dataset consisting of only several hundred samples highlights the efficiency of the LightGBM framework for data-driven composite characterisation. Unlike polynomial regression or linearised surrogate models, the gradient boosting formulation effectively resolves higher-order interactions without explicit feature engineering.

From a computational standpoint, model training times remain short, making the approach suitable for iterative design environments. Once trained, the surrogate model provides near-instantaneous predictions of equivalent shear modulus, enabling large-scale parametric exploration that would be prohibitively expensive using finite element analysis alone.

It is also observed that laminate configurations with similar global fibre angle distributions may still exhibit distinct equivalent shear moduli due to stacking sequence effects. This confirms the necessity of using a high-fidelity, data-driven surrogate rather than simplified averaging or homogenisation approaches.

Beyond forward prediction, the trained LightGBM model enables an inverse design methodology for determining laminate stacking sequences that achieve prescribed target values of equivalent shear modulus. In this inverse formulation, the surrogate model replaces the finite element solver, allowing rapid evaluation of candidate laminate configurations.

The inverse problem is posed as a minimisation task in which the absolute difference between the predicted equivalent shear modulus and a target value is minimised subject to admissible laminate constraints. The design variables consist of ply orientation angles, restricted to a predefined range consistent with manufacturing and design considerations.

A stochastic search strategy is employed to explore the design space efficiently. Candidate laminate configurations are generated by random sampling of ply angles within the allowable bounds, and the LightGBM model is used to evaluate the corresponding equivalent shear modulus. Configurations producing predictions closest to the target value are retained as optimal or near-optimal solutions.

This inverse approach is particularly advantageous for unsymmetric laminates, where classical lamination theory does not provide a direct or reliable inverse mapping between stiffness properties and stacking sequence. By leveraging the surrogate model trained on energy-equivalent finite element data, the inverse design process remains both physically consistent and computationally efficient.

Representative inverse design examples may be presented to demonstrate the ability of the method to recover multiple distinct laminate configurations yielding comparable equivalent shear modulus values. Such non-uniqueness reflects the inherent design freedom in composite laminates and further underscores the value of the proposed machine learning-based inverse framework.

Overall, the combination of finite element-based data generation, LightGBM regression modelling, and inverse laminate design constitutes a robust and scalable methodology for the determination and tailoring of equivalent shear properties in unsymmetric composite laminates.

CONCLUSION

This work presents an integrated computational and data-driven framework for the determination and inverse utilisation of an equivalent in-plane shear modulus in unsymmetric composite laminates. By combining high-fidelity finite element simulations of the ASTM D7078 V-notched rail shear test with an energy-equivalence formulation, a physically consistent definition of the equivalent shear modulus is established that remains valid in the presence of strong membrane-bending coupling and non-uniform stress fields. Unlike classical lamination theory-based closed-form expressions, the proposed approach avoids restrictive kinematic assumptions and relies exclusively on global energetic consistency, ensuring applicability to a broad class of asymmetric laminate configurations.

A fully automated data generation strategy based on NASTRAN® laminate shell modelling and systematic modification of PCOMP ply orientations enables the efficient creation of large, high-quality datasets suitable for machine learning. Among several regression algorithms evaluated, the Light Gradient Boosting Machine demonstrates the best balance between predictive accuracy and computational efficiency for the relatively small but highly nonlinear dataset characteristic of composite laminate design problems. The trained LightGBM model serves as an accurate surrogate for the underlying finite element simulations, allowing rapid forward prediction of the equivalent shear modulus and enabling inverse design studies.

Overall, the presented methodology establishes a direct and transparent link between detailed finite element simulations, energetically meaningful equivalent properties, and modern machine learning techniques. The framework is general and extensible and can be readily applied to other coupled structural-aeroelastic problems where equivalent properties are required for reduced-order modelling, preliminary design, or inverse identification. The results underline the promise of data-driven inverse methods as practical tools for the design and tailoring of advanced composite aerospace structures.

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