The inverse design and optimization for composite materials with random uncertainty

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Abstract. The inverse design is a contemporary novel modern design method and it can provide strong theoretical support for composite materials. The GMDH-NN and Kriging surrogate models are carried out to construct the transfer relations between input variables and output responses by combining finite element analysis and sensitivity analysis. In view of the objective existence of random uncertainties, structural mechanical behaviors of composite are considered as deterministic and uncertainty responses respectively, and then the corresponding optimization mathematical models are constructed. Meanwhile, genetic algorithm (GA) is employed to solve the presented inverse optimization design. Furthermore, several examples of laminated and 2D-woven composite materials are delivered to show that presented procedures are reliable and effective to obtain the dispersive of input parameters, which are of great significance in practical engineering.

1. Introduction

Since composite material has superior mechanical characteristics, such as lightweight, high strength and good stiffness etc, composite material plays an important role in aerospace, automotive industry, mechanical manufacturing and other modern engineering fields[1]. Therefore, the research on properties of composite material is a hot topic in materials science and technology. Traditionally, through constitutive relations or physical models, the expected mechanical properties can be obtained by mechanical design and optimization with complete input parameters. However, due to the inherent uncertainty factors of material, it is difficult to draw accurate conclusions in many cases. Then, it is necessary to understand the influence of random factors on mechanical behaviours for design and application. Therefore, the inverse design is a logical necessity of deepening the development of design theory and methods. Generally, an inverse design refers to the identification or designs some initial parameters by using the experimental observation data. Inverse design theory and methods are increasingly concerned in practical engineering applications, such as the geometric inverse design of airfoils according to the pressure distribution[2]. In the composite material field, the structural responses are used to deduce the inherent material characteristics according to mechanical principle, so as to obtain the optimized mechanical property distribution and achieve the stiffness or strength design indices. An inverse simulation can be used to determine input factors under the condition that the experimental results of mechanical performance are known. On the one hand, inverse design and optimization can realize the prediction of input parameter with only a small amount of performance data, which can effectively reduce the costs of time-consuming experiments. On the other hand, it can verify the accuracy of the stiffness or strength experiments and provide strong theoretical support as
well. Therefore, the significance of inverse design for composite material is not only to improve the mechanical performance, but also to bring new ideas and broader prospects for the application and manufacturing of composite materials.

So far, there are some researches on composite material inverse problems. Hu et al.[3] demonstrated a theoretical method for inverse heat transfer function in composite materials and proved the effectiveness of corrosion reconstruction. Mirzaeifar et al.[4] used inverse eigenvalue problem for computing the required changes in laminated composite plates in order to achieve desired dynamic characteristic. Visscher et al.[5] obtained the stiffness and damping properties of orthotropic composite plates by comparing the experimental parameters with the corresponding results of the modal strain energy method. Besides, Antonio et al.[6] used probabilistic models to estimate reliability level by inverse reliability-based design optimization via Artificial Neural Network (ANN).

In general, there is no analytical solution for most practical engineering problems. And the numerical simulation is very time-consuming. Furthermore, it is difficult to achieve the unique and stable solutions of inverse process for the complexity of composites and numerous random factors[7]. With the development of computer aided engineering techniques, inverse design method integrated with modern intelligent techniques can be an extensive application recently. With the assistance of finite element simulation, the inverse optimization design based on surrogate methods is proposed to obtain the dispersive of input parameters for laminated and 2D-woven composite material. Genetic algorithm and sensitivity analysis also play important roles in optimizing process.

The remaining of this paper is organized as follows: Section 2 illustrates the establishment of transfer function between input parameters and output mechanical behaviours with the aid of finite element analysis and advanced surrogate model technology. The methodology of composite inverse design for deterministic and random problems is described in Section 3. Section 4 provides inverse design tests of laminated and 2D-woven composite materials, and validates the adaptability of the proposed method respectively. Finally, conclusions are drawn in Section 5.

2. The transfer function of composite materials

2.1. Finite element analysis of composite materials

For the small deformation problems of composite laminates and woven unit cells, the finite element method (FEM) is a universal method and a helpful assistance in inverse design. The smoothed particle hydrodynamics (SPH)[8] or Lagrangian gradient smoothing method (L-GSM)[9] can be used to analyze the dynamic problems with high mesh quality requirements. ABAQUS modeling and analysis are worldwide used to analyze dynamic or static responses of nonlinear structure and material[10]. The pre-modeling streamline mainly contains establishing geometry units, assigning metal or composite material properties, meshing, setting loading environment and submitting to solver. The post-processing is conducted through ABAQUS/standard to obtain mechanical behaviors such as stress/strain or transformed stiffness and strength. In the iterative optimization process, the finite element model needs to be reconstructed by adaptive parametric modeling. With the help of the kernel Python script language, the construction of composite structures becomes more concisely and flexibly. There is another woven material modeling software, TexGen package, which will be discussed in subsection 2.1.2.

2.1.1. Finite element simulation of laminated composites. Laminated composite is composed of ply-up single lamina, whose mechanical properties can be obtained from tensile and shear tests. 2D layup plates are the most common form of composite laminates, and their properties can be comparatively accurately integrated on grid points by Quad type meshes in ABAQUS. Layup patterns can be set in Composite Layup Module through graphical user interface (GUI) and it is available to view the settings of each layer through query commands. The general modeling operations are shown in Figure 1. This procedure can also be achieved by Python script via parameter tuning such as the stacking sequence, layer thickness and ply orientation. Since ABAQUS can record the operating flow of the
modeling process, the simplest compile method is a semi-parametric modeling through the combination of the command stream and Python script. The maximum displacement of laminated structure can be determined as mechanical output and its value can also be obtained by Python in ABAQUS field-output module.

**Figure 1.** The modeling process of laminates in ABAQUS.

### 2.1.2. Finite element simulation of 2D-woven composites.

The geometric of fabric unit cell is constructed by TexGen package. TexGen (developed by Nottingham University) can quickly permit the realization of parametric modeling of woven composite unit cell or a representative volume element (RVE) automatically. The modeling method is carried out to first specify a series of nodes on the yarn trajectory, establish yarn central axis through interpolation curve, and generate the unit model by sweeping the cross-section contour, and eventually expand in three directions to obtain 3D model. Besides, the Python script can be programmed within ABAQUS by integrating the TexGen Python modules[11]. Modification of input parameters and FEA calling can be achieved by MATLAB, which is also used for post-processing and data analysis.

![Cross-section parameters of a twill unit cell](image)

**Figure 2.** Cross-section parameters of a twill unit cell.

TexGen can create a variety of different textile composite models. Considering the same warp and weft yarns of 2D twill composites, three-dimension eight-node brick element with reduced integration (C3D8R) are used in the woven cell, and there are mainly three independent geometric parameters to control cell shape, including yarn width W, fabric thickness H and yarn space S (shown in Figure 2).

The variability of parameters will further affect material behaviors, such as yarn crimp, fiber volume fraction, and ultimately affect the macro-mechanical properties of composites[12].

### 2.2. Surrogate model of composite material

The relation between input variables and output response is depicted in Figure 3. It needs a large number of analytical formulas or multiple finite element simulation to construct an explicit transfer relation function \( g(X) \). Therefore, surrogate models are introduced to construct \( g(X) \) with less computational time.

Several robust surrogate methodologies have been developed nowadays. Modified Group Method of Data Handling-Neural Network (GMDH-NN) method[13] and Kriging methodology[14] are employed to substitute the transfer function \( g(X) \) of laminates and woven composites respectively.
The material parameters, geometric parameters, stacking sequence, loading characteristics of the lamina, etc.

Calculation of stiffness and compliance matrices

Finite element analysis

Tensile, compressive and shear performances etc.

**Figure 3.** The relationship between input parameters and output response.

### 3. Inverse design model and optimization process

The aim of inverse design is to find input parameters by inverse simulation on condition that the performance data of experimental mechanical behaviors are given. The distribution characteristics (distribution type, mean, variance, etc.) of geometric and material properties can be known from a large number of experimental samples. However, it is difficult to obtain complete statistical information of mechanical response through small experimental samples. The finite element analysis (FEA) is employed to simulate the input-output relationship in ideal experimental state. Import random samples into simulation models and submit to software solver, then simulated mechanical behavior or stiffness can be obtained. Then, surrogate models can be employed to greatly reduce the number of finite element analysis. By minimizing the difference between the authentic statistics and the simulated structural response, i.e. searching for the simulated distribution closest to true responses, we can derive the optimal input information iteratively through inversed transfer function $g^{-1}(X)$ expressed by surrogate models. The applicability of the proposed method can be used in both deterministic and random problems.

#### 3.1. The inverse design for deterministic problems

When the known information is only a single experimental data or design target value, one or a set of deterministic input variables can be obtained through optimization. Firstly, classify input variables $x = (x_{\text{var}}, x_{\text{in}}, x_{\text{sic}})$, and $x_{\text{var}}, x_{\text{in}}$ are unknown and known deterministic variables, $x_{\text{sic}}$ are random variables. Then, acquire structural response $y$ (displacement, stress, etc.) of experimental samples. The inverse simulation mathematical models can be constructed.

$$\begin{align*}
\text{find } \theta \text{ of } x_{\text{var}} \\
\min d = |\beta - \beta^*| \\
s.t. \ y = g \left( x_{\text{var}}, x_{\text{in}}, x_{\text{sic}} \right)
\end{align*}$$

where $\theta$ is denoted as the distribution parameters of input variable, $d$ refers to the differences between authentic statistical properties and structural output response, $\beta$ is defined as the reliability index (the ratio of mean and standard deviation in standard normal space) of real properties, $\beta^*$ is the reliability index of simulated output response. Particular constraints such as boundary conditions and deformation limits must be added for different loading cases.

#### 3.2. The inverse design for random problems

For random problems, so far there is no way to deduce the complete input uncertain distribution from a general output uncertain distribution. Therefore, we only consider the case that the prior distribution type of input variables are known and the task is to find the optimal random parameters. When given multiple test data or a range of design intervals, the statistical characteristics of input variables can be obtained through inverse design, and then the distribution parameters of each variable can be derived.
As long as the distribution of experimental data is obtained, we made an improvement on the basis of minimizing the sum of square errors in reference [4], the optimal inverse model for uncertainty response is established as follows:

\[
\text{find } \theta \text{ of } \mathbf{x}_{\text{nei}} \\
\min \, D = \sum_{j=1}^{2L} \sum_{i=1}^{2L} \| M_{ij}^{*} - M_{ij}^* \| (j = 1, 2L \, \, n, i = 1, 2L \, \, m)
\] (2)

where \( D \) is denoted as the difference of first \( n \)-order statistical moments between real properties and structural output response. The similarity between real values and simulation distribution is represented by moments (usually first four-order moments). That is to say, \( M_{ij}^{*} \) is the moment of real properties, \( M_{ij}^* \) is the moment of output response. Its minimization process is based on the convergence criteria of the selected optimization algorithm. When the differences between statistical moments reach the minimum, the corresponding distributions of input variables are the optimal solution.

In addition, Genetic algorithm (GA) is a popular optimization and search technique based on the principles of genetics and natural selection[15]. It is a highly parallel global randomization search algorithm, which can automatically acquire and accumulate knowledge about search space and adaptively control the search process to obtain the optimal solution. Due to the powerful ability for solving nonlinear engineering problems, GA is used to solve the global optimal of the presented inverse design problems. The complete schematic of the basic idea for the proposed inverse design method of deterministic and random problems with GA optimization can be depicted by Figure 4.

4. Tests and analysis

4.1. Laminate test

In practical engineering, laminated plates are always considered as thin plates, the implementation of the finite element method follows the classical lamination theory (CLT).

Now consider an I-section composite cantilever beam with fixed end is subject to uniformly distributed load \( P = 0.1 \text{MPa} \) perpendicular to the upper surface[16]. The cross-section size of composite beam is illustrated in Figure 5. The stacking sequence of upper and lower board is \([45^\circ/-45^\circ/0^\circ/90^\circ]\), and \([45^\circ/-45^\circ/-45^\circ/45^\circ]\), in web plate. The thickness of a single layer is 0.25mm. Regard all material parameters as independent normal input variables, take the coefficient of variation (Cov) as 0.06, the objective function of minimizing the maximum displacement of the cantilever beam is carried out, advanced GMDH-NN is employed to construct the transfer model (the displacement nephogram is shown in Figure 6). The errors set out in Table 1 are generally not more than 6\%, which can achieve the engineering calculation requirements.

4.2. Twill composite test

For two-dimensional woven materials, the geometry modeling is based on these reasonable assumptions: (1) The shape function of yarns is idealized as a periodic sine function curve; (2) The warp and weft yarns with the same performance are orthogonal and full contacted; (3) The elliptical cross-section of yarns remains unchanged along the yarn path.

The 2x2 twill cell simulated in TexGen and its fiber meshes in ABAQUS is depicted in Figure 7. The model is analyzed by calling ABAQUS solver in MATLAB and extracting the reaction force information of nodal points in the post-processing *.odb file of ABAQUS to obtain modulus with numerical calculations combined.
Ideal objectives or experimental data
Transfer relation: \( g(x) = y \)

Find the difference of reliability index
Initial design parameters

Deterministic problems
Find the difference of the first four moments

Random problems

GA optimization

If \( d \) is minimum?

No

Yes

If \( D \) is minimum?

No

Yes

Stop iteration

Figure 4. The schematic of presented inverse design method with GA.

Figure 5. The section sketch of composite beam.  
Figure 6. The displacement of composite beam.

Table 1. The inversed result with comparison to truth value for composite beam.

| Material parameters | \( E_{xx} \) (GPa) | \( E_{yy} \) (GPa) | \( G_{xy} \) (GPa) | \( \nu_{xy} \) |
|---------------------|-----------------|-----------------|-----------------|---------------|
| Truth value         | 135.000         | 8.800           | 4.470           | 0.330         |
| Presented method    | 138.310         | 9.328           | 4.738           | 0.318         |
| (Error)             | (2.45%)         | (6.00%)         | (6.00%)         | (3.64%)       |

Figure 7. Twill cell model in TexGen (left) and fiber meshes in ABAQUS (right).
According to NASA scholars’ previous research [17], on the probabilistic model of woven composites, it can be presumed that the parameters of the fiber and the matrix material are independent with each other and obey the normal distribution. Moreover, Cov of geometric parameters is 0.1. And there are normal variables $E_{11}$, $E_{22}=E_{33}$, $G_{12}=G_{13}$, $\nu_{12}=\nu_{13}$, $\nu_{23}$, $G_{23}$ for fiber and $E_{m}$ and $\nu_{m}$ for matrix to be considered with Cov equals to 0.05. The geometric and material properties are given in Table 2.

In order to observe the influence of uncertainty factors more intuitively, three cases are considered: 1) the material properties are random factors, 2) geometric properties are random factors, 3) material and geometry properties exist uncertainties at the same time. The probability density function (PDF) of their mechanical response $E_x$ under above cases can be fitted by kernel density estimation (KDE), and the comparison with the ideal normal distribution can be shown in the Figure 8.

Table 2. Geometric and material properties of twill model.

| Parameters | Mean | Parameters | Mean |
|------------|------|------------|------|
| Geometric  |      | Carbon fiber |      |
| $H$        | 0.2mm| $E_{11}$   | 220.690 GPa |
| $W$        | 0.8mm| $E_{22}=E_{33}$ | 13.790 GPa |
| $S$        | 0.2mm| $\nu_{12}=\nu_{13}$ | 0.200 |
|            |      | $\nu_{23}$ | 0.250 |
| Epoxy      |      | $G_{12}=G_{13}$ | 8.970 GPa |
| matrix     | 3.100 GPa | $G_{23}$ | 4.830 GPa |
| $E_m$      |      | $\nu_m$ | 0.390 |

It can be seen from Figure 8 that PDF of output response $E_x$ will deviate from the ideal normal distribution when considering uncertain factors. In practical engineering problems, there are often a lot of objective uncertainties, and it is more accurate to predict the actual results with full and reasonable consideration of these uncertainties.

Figure 8. PDF of $E_x$ with random uncertainty under three cases.

Again, take longitudinal Young’s modulus $E_{xx}$ as an example, there is only about 4% error between predicted elastic property (59.27GPa) through FEA and the literature result (56.97GPa) [17]. The sensitivity analysis results of geometric and material input parameters for elastic property are shown in Table 3.

Table 3. Sensitivity analysis of input parameters to elastic property $E_{xx}$.

| $E_{11}$ | $W$ | $H$ | $S$ | $G_{23}$ | $\nu_{12}$ | $E_{33}$ | $E_m$ | $\nu_{23}$ | $\nu_m$ | $G_{12}$ |
|----------|-----|-----|-----|---------|------------|---------|-------|------------|--------|---------|
| 0.4403   | 0.2635 | 0.0709 | 0.0633 | 0.0064       | 0.0047         | 0.0042 | 0.0033 | 0.0029        | 0.0025 | 0.002   |
To reduce dimensionality of input variables, 97% of the total contribution are regarded as important variables. The sensitivity analysis shows that the material parameter of yarn $E_{11}$ contribute the most to the equivalent tensile modulus $E_{xx}$, followed by geometric variables $W$, $H$ and $S$. By using Kriging model to construct transfer function, we obtained the distribution of inversed input variables through genetic algorithm optimization. The predicted input unit cell geometric and material parameters of $E_{xx}$ are shown in Table 4. The presented method shows that the inversed input variables are within reasonable error ranges, and Kriging model integrated with GA shows well adaptability composite parameter inverse problems.

### Table 4. The inversed input variables with Kriging method for $E_{xx}$

|            | $E_{11}$ (GPa) | $S$ (mm) | $H$ (mm) | $W$ (mm) |
|------------|----------------|----------|----------|----------|
| Truth value| 220.69         | 0.2      | 0.2      | 0.8      |
| Presented method (Error) | 223.7257 (1.38%) | 0.196531 (1.73%) | 0.19702 (1.49%) | 0.759273 (5.09%) |

### 5. Conclusion
This paper presents a novel inverse design and optimization procedure for laminated and 2D-woven composite material. Advanced surrogate models can efficiently replace the direct finite element method. Sensitivity analysis can reduce the dimensionality of input variables. GA is carried out to solve the inverse optimization models. Laminated and 2D-woven composite material examples are tested to validate the feasibility of inverse design. The following conclusions can be drawn:

1) For deterministic problems, a set of deterministic input variables can be inversed by minimizing the differences of reliability indices between experimental value and FEM results. Laminated composite test shows the proposed method can estimate the geometric and material parameters accurately.

2) For random problems, the statistical characteristics of input variables can be inversed. By minimizing the first four order moments between simulated and truth test values, the distribution of input random parameters can be found.

Taking the inhere uncertainty into consideration, the authenticity of inverse design can be further enhanced by fully mining experimental and simulation data.

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