Data-driven topology optimization (DDTO) for three-dimensional continuum structures

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Abstract
Developing appropriate analytic-function-based constitutive models for new materials with nonlinear mechanical behavior is demanding. For such kinds of materials, it is more challenging to realize the integrated design from the collection of the material experiment under the classical topology optimization framework based on constitutive models. The present work proposes a mechanistic-based data-driven topology optimization (DDTO) framework for three-dimensional continuum structures under finite deformation. In the DDTO framework, with the help of neural networks and explicit topology optimization method, the optimal design of the three-dimensional continuum structures under finite deformation is implemented only using the uniaxial and equi-biaxial experimental data. Numerical examples illustrate the effectiveness of the data-driven topology optimization approach, which paves the way for the optimal design of continuum structures composed of novel materials without available constitutive relations.

Keywords Data-driven · Topology optimization · Three-dimensional continuum structures · Finite deformation · Constitutive model-free

1 Introduction

Structural topology optimization aims to find the optimal material distribution under prescribed objective functions and constraint conditions in the design domain. Since the pioneering work of Bendsøe and Kikuchi (1988), topology optimization of the continuum structure has received a lot of interest from researchers and engineers. Nowadays, many structural topology optimization methods have been proposed, such as the solid isotropic material with penalization (SIMP) method (Bendsøe 1989; Zhou and Rozvany 1991), the level set method (LSM) (Wang et al. 2003; Allaire et al. 2004), the evolutionary structural optimization (ESO) method (Xie and Steven 1993), the moving morphable components (MMC) method (Guo et al. 2014), etc. Although significant progress has been achieved in the optimal design of continuum structures, most research is carried out under the linear elasticity and small deformation assumptions, which inevitably restrict the applications.

In terms of the topology optimization of continuum structures with material and geometric nonlinearities, some excellent progress has been reported recently. Based on the LSM, Chen et al. (2017) designed hyperelastic structures undergoing large deformation. Dalklint et al. (2020) studied the eigenfrequency constrained topology optimization of hyperelastic structures. Deng et al. (2019) presented a topology optimization method based on distortion energy for designing hyperelastic material against failure. Recently, topological design of porous infill structures with hyperelastic material under large deformation configurations was reported in Huang et al. (2022). Using a modified...
evolutionary topology optimization method, Zhang et al. (2020a) maximized the stiffness of hyperelastic structures in the finite deformation regime. Silva et al. (2020) proposed a modified Normal Distribution Fiber Optimization (NDOI) model to perform topology optimization of fibers orientation in composites. Based on the hyperelasticity theory, Zhang et al. (2020b; Zhang and Chi 2020) implemented the structural topology optimization design of multi-material and local feature control, respectively. It is worth noting that various techniques which alleviate the convergence difficulties caused by the excessive distortion of low-density elements, play a vital role in the topology optimization of continuum structure with geometric nonlinearity, e.g., see Buhl et al. (2000), Yoon and Kim (2007, 2005), Lahuerue et al. (2013), Wang et al. (2014), Ha and Cho (2008), Xia and Shi (2016), Luo et al. (2015), Dijk et al. (2014), and Xue et al. (2019) for reference.

It is worth mentioning that, all of the studies mentioned above were investigated under the constitutive model-based structural topology optimization framework. On the one hand, developing a matured analytic function-based constitutive model, in general, is very demanding; on the other hand, there may be no available accurate constitutive models for new materials, such as many synthetic polymers and additive manufactured materials. To be specific, reference Tang et al. (2019) shows that the neo-Hookean model, Arruda–Boyce model, and Odgen model cannot capture the mechanical property accurately under compression and/or tension for fabricated silicone rubber. For some detailed data, please refer to Tang et al. (2019). At this circumstance, it would be extremely difficult to design optimal structures only with the collection of experimental data of such materials. Fortunately, Kirchdoerfer and Ortiz (2016) proposed a data-driven computational mechanics (DDCM) framework, which realized structural mechanics analysis based only on experimental material data. Later works suggested performing the DDCM based on locally characterizing the material constitutive behavior to accelerate the global data-driven solver and improve the robustness against noise (Ibañez et al. 2017, 2018; He and Chen 2020; Kanno 2018). To consider the inevitable multi-source uncertainties in the material data set, Guo et al. (2021) proposed an uncertainty analysis-based data-driven computational mechanics (UA-DDCM) framework to obtain a solution set rather than a specific value of the concerned structural response. Tang et al. (2019, 2020, 2021) and Chen et al. (2022) developed a so-called MAP123 method based on the principle of mechanics. They successfully realized the mechanical analysis of the three-dimensional structures only using experimental material data of uniaxial tension, or uniaxial and equi-biaxial tension. In addition, in terms of constitutive construction with artificial neural networks, Masi et al. (2021) proposed thermodynamics-based artificial neural networks for constitutive modeling, and Bonatti and Mohr (2022) established a constitutive model of elastoplastic materials by using recurrent neural networks. More relevant works can be found in the references therein.

Inspired by the success of data-driven computational mechanics, the idea of data-driven topology optimization (DDTO) emerges naturally (Zhou et al. 2020), which aims at designing optimal structures with no available constitutive laws and only using experimental data. To the best of our knowledge, under the small deformation assumption, the only DDTO work was reported by Zhou et al. (2020), which focused on topology optimization of truss structures (only requires uniaxial experimental data) and adopted the classic data-driven analysis algorithm in Kirchdoerfer and Ortiz (2016).

Besides the novel and encouraging results achieved in the work (Zhou et al. 2020), extending such DDTO approach to design three dimensional continuum structures could be quite challenging: (1) a sufficient data set of three dimensional constitutive relation under finite deformation would be huge and difficult to collect; (2) due to the huge amount of data, the bi-level programming of the classic DDCM framework could be very expensive; (3) the complex stress state and excessive deformation make the convergence of analyzing continuum structures (especially intermediate structure in design process) more difficult than the analysis of truss structures in small deformation regime.

To address the above issues, in the present work, a mechanistic-based data-driven topology optimization (DDTO) framework for three-dimensional continuum structures is proposed. A new data-driven analysis algorithm, i.e., the improved MAP123 method, is adopted for structural analysis. Under this circumstance, only the uniaxial and equi-biaxial experimental data are required, and the classic Newton–Raphson iterative algorithm guarantees the efficiency and robustness of the data-driven analysis algorithm. Besides, taking the advantage of the decoupling of geometry model and analysis model in the MMV method, the degree of freedom of low-density elements can be eliminated to further improve the numerical stability of structural analysis.

The remainder of the paper is organized as follows. In Sect. 2, the classical constitutive model-based topology optimization framework for three-dimensional hyperelastic continuum structures under finite deformation and the corresponding solution strategies are explained. In Sect. 3, after developing a stable data-driven analysis method for three-dimensional continuum structures, the DDTO framework, its sensitivity analysis and solution strategy are presented. After numerical examples illustrating the effectiveness of the DDTO framework in Sect. 4, some concluding remarks are provided in Sect. 5.
2 Constitutive model-based explicit topology optimization framework for three-dimensional hyperelastic continuum structures under finite deformation

For completeness, this section mainly introduces the classical constitutive model-based topology optimization (CMTO) framework for three-dimensional hyperelastic continuum structures, including subsections about the three-dimensional Moving Morphable Void (MMV) method, problem formulation, and numerical solution strategies.

2.1 Three-dimensional Moving Morphable Void (MMV) method

To solve the topology optimization problems of linear elastic three-dimensional continuum structures, Zhang et al. (2017) proposed the so-called 3D-MMV method. As shown in Fig. 1a, an optimized structure is described by a set of movable and morphable voids in Fig. 1a, an optimized structure is described by a set of movable and morphable voids. The schematic diagram of the 3D-MMV method, an optimized structure, b geometry representation of the ith void. The coordinate of its center, as illustrated by Fig. 1b, \( \theta \) and \( \varphi \) are the azimuths, \( r(\theta, \varphi) \) is the distance function from the point on the boundary \( \partial \Omega \) to the center point of the void and its detailed expression is listed in Appendix A.

Based on Eq. (2.1), the global TDF of the whole structure can be constructed as (Du et al. 2022):

\[
\chi^i(D; x) = \min_{i=1, \ldots, m_V} \chi^i(D^i; x) \approx \frac{1}{-\lambda} \ln \left( \sum_{i=1}^{m_V} e^{-\lambda \chi^i(D^i; x)} \right),
\]

where \( D^i = \left( C_{x_i}^i, C_{y_i}^i, C_{z_i}^i; r_{0, l_i}, r_{0, l_i} \right) \), \( k = 1, \ldots, K, l = 1, \ldots, L - 1 \), and \( \lambda \) is a relatively large even number, e.g., \( \lambda = 80 \). Notably, the design variable vector in the MMV approach is \( D = \left( \left( D^1 \right)^T, \ldots, \left( D^{m_V} \right)^T \right)^T \) and it only contains geometrically explicit parameters.

2.2 Problem formulation

By adopting the total Lagrangian formulation, for minimum end compliance design problems, the constitutive model-based explicit topology optimization framework for three-dimensional hyperelastic continuum structures can be formulated as:

Find \( D = \left( \left( D^1 \right)^T, \ldots, \left( D^{m_V} \right)^T \right)^T, 0 u(D; 0 x) \), Minimize \( J(D, 0 u) = \int_{\Omega} \bar{H}_e \left( \chi^e(D_i; 0 x) \right)^T 0 F \cdot 0 u d^3 V + \int_{\partial \Omega_k} \bar{t}_l \cdot 0 u d^2 S \),

S. t.
\[
\int_{\Omega} H_e^a (\chi^a(D,0) x) \delta F^T : P d^0 V = \int_{\Omega} H_e^a (\chi^a(D,0) x) 0_f \cdot \delta^0 u d^0 V + \int_{\delta S} 0_t \cdot \delta^0 u d^0 S, \forall 0 u \in \mathcal{U}_d.
\]

\[
\int_{\Omega} H_e^a (\chi^a(D,0) x) d^0 V \leq 0 V,
\]

\[D \subset \mathcal{U}_d,\]

\[0 u = 0, \text{ on } 0 S_u,\]  

(2.3)

where \(I(D,0 u)\) is the end compliance of the optimized structure, \(\Omega\) is the undeformed design domain and \(0(\cdot)\) denotes the variables in the initial configuration. The 1st Piola–Kirchhoff stress tensor \(P\) is obtained from the Cauchy stress tensor \(\sigma\) determined by the strain energy density function \(W\) (see Sect. 3), i.e., \(P = J \sigma \cdot F^{-T}\) with \(F\) and \(J\) denoting the deformation gradient and the determinant of \(F\). Besides, \(0 f\) is the body force density, \(0 u\) is the displacement field of the structure, \(\delta^0 u\) is virtual displacement, \(0 t\) is surface tractions density, \(\mathcal{U}_d\) is the admissible set that \(\delta^0 u\) belongs to, \(0 S_u\) is the Dirichlet boundary, \(0 V\) is the upper bound of admissible solid material. The regularized Heaviside function \(H_e^a\) is expressed as

\[
H_e^a (x) = \begin{cases} 
1, & \text{if } x > \epsilon, \\
\frac{3(1-a) x - x^3}{4 \epsilon^3}, & \text{if } -\epsilon \leq x \leq \epsilon, \\
\alpha, & \text{otherwise,}
\end{cases}
\]

(2.4)

where \(\epsilon\) is the width of regularized region and \(\alpha\) is a small positive number, which are set as 0.1 and 10^{-3}, respectively. In the solution process of formulation (2.3), the strain energy density function \(W_e\) of the hyperelastic material corresponding to the \(e\) th element is obtained according to the ersatz material model as

\[
W_e = \rho_e W_0 = \sum_{i=1}^{nn} H_e^a (\chi^a(D,0) x) e^i W_0.
\]

(2.5)

where \(\rho_e\) is the density of the \(e\) th element, \(nn\) is the total number of the nodes in \(e\) th element, \(\chi^a(D,0) x\) is the \(i\) th nodal value of the global TDF of the \(e\) th element, \(W_0\) is the strain energy density functional of the base material.

### 2.3 Numerical solution strategies

#### 2.3.1 Redundant degrees of freedom removal technique

The solution process of topology optimization of three-dimensional hyperelastic continuum structures under finite deformation usually encounters the non-convergence issue of the finite element analysis caused by the excessive deformation of weak material elements. The so-called redundant degrees of freedom removal technique (Xue et al. 2019; Zhang et al. 2017; Du et al. 2022) is adopted to alleviate this issue. The core idea of this technique is to remove the degrees of freedom (DOFs) only involved in the weak material elements which are identified by Eq. (2.6) for the nonlinear structural analysis:

\[
\rho_e = \frac{\sum_{i=1}^{nn} H_e^a (\chi^a(D,0) x) e^i}{nn} \leq TR,
\]

(2.6)

where \(TR\) is a threshold taken as 0.1 in the present work. It is worth noting that, thanks to the decoupling between the geometry description and finite element analysis, one would not need to worry about the reintroduction of the removed DOFs in subsequent iterations. For some more detailed explanations, please refer to Xue et al. (2019), Zhang et al. (2017), and Du et al. (2022).

#### 2.3.2 Finite element analysis

Combining the weak form of the balance equation in Eq. (2.3) and the redundant degrees of freedom removal technique, the balance equation of the retained degrees of freedom in the design domain can be written as:

\[
\tilde{R}(D,\tilde{U}) = \tilde{f}^{\text{int}} - \tilde{f}^{\text{ext}} = \sum_{e=1}^{Rne} L_{pe}^{T} f_{e}^{\text{int}} - \sum_{e=1}^{Rne} L_{pe}^{T} f_{e}^{\text{ext}} = 0,
\]

(2.7)

where \(\tilde{U}, \tilde{R}(D,\tilde{U}), \tilde{f}^{\text{int}}\) and \(\tilde{f}^{\text{ext}}\) are the displacement vector, the residual force vector, the internal force vector and the external force vector of the retained DOFs in the design domain, respectively. The symbol \(Rne\) is the number of the elements with density larger than the threshold in the design domain, and \(L_{pe}\) is the connection matrix of the \(e\) th element. The internal force vector \(f_{e}^{\text{int}}\) and the external force vector \(f_{e}^{\text{ext}}\) of the \(e\) th element can be expressed as:

\[^1\] While in the 3D case, more DOFs related to low-density element need to be eliminated to solve the convergence issue caused by excessive deformation of low-density elements. Thanks to the decoupling of the geometry model and analysis model in the MMV method, we won’t need to worry about the reintroduction of removed DOFs or elements in subsequent iteration (Xue et al. 2019; Zhang et al. 2017; Du et al. 2022).
\[ J^\text{int} = \int_{\Omega_u} B^T P d^e V_e J^\text{ext} = \int_{\Omega_u} N^T \delta f d^e V_e + \int_{\Sigma_S} N^T \delta d^h S, \]  
(2.8)

where \( B \) is the operation matrix between \( \delta F \), and the virtual displacement \( \delta U_e \), \( N \) is the shape function matrix. Implementing the Newton–Raphson algorithm, the displacement vector \( \tilde{U}^{k+1} \) at the \( k \) th iteration is updated as

\[
\begin{align*}
K_T(D, \tilde{U}^k) \Delta U = -\tilde{R}(D, \tilde{U}^k) & = J^\text{ext} - J^\text{int}(D, \tilde{U}^k), \\
\tilde{U}^{k+1} = \tilde{U}^k + \Delta U,
\end{align*}
\]
(2.9)

where \( K_T(D, \tilde{U}^k) \) and \( \Delta U^k \) are the tangent stiffness matrix and the nodal displacement at the \( k \)th iteration. If \( \|\tilde{R}(D, \tilde{U}^k)\| < \delta \) with \( \delta \) denoting a prescribed small number, e.g., \( \delta = 10^{-6} \), the structure is supposed to achieve an equilibrium state.

### 2.3.3 Sensitivity analysis

Without the loss of generality, the body force is ignored in the present work. Based on the adjoint sensitivity analysis method, the Lagrangian function only involving the retained DOFs can be written as:

\[
L(D, \tilde{U}, \tilde{\lambda}) = f^\text{ext} \tilde{U} + \tilde{\lambda}^T \tilde{R}(D, \tilde{U}).
\]
(2.10)

where \( \tilde{\lambda} \) is the corresponding adjoint displacement vector. With Eq. (2.10) in hand, the derivative of the objective function with respect to the design variables is expressed as:

\[
\frac{\partial f(D, \delta u)}{\partial D} = \frac{\partial L(D, \tilde{U}, \tilde{\lambda})}{\partial D} = \frac{1}{mn} \sum_{c=1}^{ne} \left( \sum_{i=1}^{nn} \frac{\partial H^e_i(\chi^e_i)}{\partial \chi^e_i} \frac{\partial \chi^e_i}{\partial D} \right) \tilde{\lambda}.
\]
(2.11)

The detailed expressions of \( \frac{\partial f}{\partial D} \) are presented in Appendix B and the adjoint displacement vector can be solved by the following adjoint equation:

\[
\tilde{\lambda} = -\left(K_T(D, \tilde{U}^E)\right)^{-1} f^\text{ext},
\]
(2.12)

where \( K_T(D, \tilde{U}^E) \) and \( \tilde{U}^E \) are the tangent stiffness matrix and the displacement vector at the equilibrium state, respectively. The sensitivity result of the volume constraint is:

\[
\frac{\partial V}{\partial D} = \frac{1}{mn} \sum_{c=1}^{ne} \sum_{i=1}^{nn} \frac{V_e}{V_D} \frac{\partial H^e_i(\chi^e_i)}{\partial \chi^e_i} \frac{\partial \chi^e_i}{\partial D},
\]
(2.13)

where \( ne \) is the total number of elements in the structure, the symbols \( V_e \) and \( V_D \) are the volumes of the \( e \)th element and the design domain, respectively.

### 3 The DDTO framework for three-dimensional continuum structures under finite deformation

In this section, firstly, a stable data-driven structural analysis (DDSA) algorithm for three-dimensional continuum structures under finite deformation is proposed. Then the effectiveness of DDSA algorithm is verified by a numerical example. Finally, the solution techniques of the corresponding DDTO framework are given.

#### 3.1 Neural network enhanced DDSA algorithm for three-dimensional continuum structures under finite deformation

In Tang et al. (2019) and Chen et al. (2022), a constitutive model-free DDSA algorithm for three-dimensional hyperelastic continuum structures is proposed only using the experimental data of uniaxial tension, or uniaxial and equi-biaxial tension tests. In the present work, we also assume the mechanical property of the considered material is approximately hyperelastic. To improve the robustness of the algorithms in Tang et al. (2019) and Chen et al. (2022) for intermediate structures in the optimization process, here, an improved DDSA algorithm, which additionally uses the experimental data of uniaxial compression and equi-biaxial compression test, is proposed. Furthermore, an artificial neural network-based stress update strategy is proposed to ensure the stability and robustness of the structural analysis.

#### 3.1.1 The prior knowledge in mechanics

For an isotropic hyperelastic material, its mechanical behavior can be characterized by a strain energy density function expressed as:

\[
W = W(\tilde{I}_1, \tilde{I}_2, J),
\]
(3.1)

where \( \tilde{I}_1 = \text{tr} (\tilde{b}) \) and \( \tilde{I}_2 = \frac{1}{2} [\tilde{I}_1^2 - \text{tr} (\tilde{b} \cdot \tilde{b})] \) are the first and second invariants of \( \tilde{b} \), respectively. The symbol \( \tilde{b} = \tilde{F} \cdot \tilde{F}^T \) is the modified left Cauchy-Green tensor and \( \tilde{F} = J^{-\frac{1}{3}} F \) is the modified deformation gradient with the volume change eliminated. The Cauchy stress can be derived as:

\[
\sigma = \frac{2}{J^{\frac{1}{3}}} \left( \frac{\partial W}{\partial \tilde{I}_1} + \tilde{I}_1 \frac{\partial W}{\partial \tilde{I}_2} \right) \tilde{b} - \frac{2}{J^{\frac{2}{3}}} \frac{\partial W}{\partial \tilde{I}_2} \tilde{b}^2
+ \left( \frac{\partial W}{\partial J} - \frac{2}{3J} \frac{\partial W}{\partial \tilde{I}_1} \right) J.
\]
(3.2)
where \( \mathbf{I} \) is the second order identity tensor and \( \mathbf{b} = \mathbf{F} \cdot \mathbf{F}^\top \) is the left Cauchy-Green tensor. Furthermore, the spherical part and the deviatoric part of the Cauchy stress can be obtained as:

\[
\sigma_m = \frac{\partial W}{\partial \mathbf{J}},
\]

\( (3.3a) \)

\[
\text{dev}(\mathbf{\sigma}) = \gamma \text{dev}(\mathbf{b}) + \beta \text{dev}(\mathbf{b}^2),
\]

\( (3.3b) \)

where \( \gamma = \frac{2}{3} \left( \frac{\partial w}{\partial \mathbf{e}} + \mathbf{I}^\top \frac{\partial w}{\partial \mathbf{e}} \right) \), \( \beta = -\frac{2}{3} \frac{\partial w}{\partial \mathbf{e}} \), and \( \text{dev}(\cdot) \) denotes the deviatoric operator.

It is clear that, uniaxial and equi-biaxial experimental data are sufficient for determining the spherical part of the Cauchy stress. However, due to the complexity of the deviatoric part of the Cauchy stress in high dimensions, it is impossible to represent the material property information of the entire state space by only using the uniaxial and equi-biaxial experimental data. This motivates us to reconstruct the deviatoric part of the Cauchy stress with the help of material parameters \( \gamma \) and \( \beta \).

To determine the material parameters \( \gamma \) and \( \beta \), the equivalent Cauchy stress \( \sigma_e \) and equivalent strain \( \mathbf{b}_e \) are defined as:

\[
\sigma_e = \sqrt{\frac{3}{2} \text{dev}(\mathbf{\sigma}) : \text{dev}(\mathbf{\sigma})},
\]

\( (3.4a) \)

\[
\mathbf{b}_e = \sqrt{\frac{2}{3} \text{dev}(\mathbf{b}) : \text{dev}(\mathbf{b})}.
\]

\( (3.4b) \)

Combining Eqs. (3.4a), (3.4b) and (3.3b), we have

\[
\frac{2}{3} \sigma_e^2 = \frac{3}{2} \gamma \sigma_e^2 + 2\gamma \beta \mathbf{b}_e^2 + \frac{\beta}{3} \text{dev}(\mathbf{b}) : \text{dev}(\mathbf{b}) + \beta \text{dev}(\mathbf{b}^2) : \text{dev}(\mathbf{b}^2).
\]

\( (3.5) \)

Generally, the strain energy density function \( W \) of a hyperelastic material includes two cases: (1) \( W \) is dependent on \( \mathbf{I}_1, \mathbf{I}_2 \), and \( \mathbf{J} \), e.g., the Mooney-Rivlin and Van der Waals models, and (2) \( W \) is only dependent on \( \mathbf{I}_1, \mathbf{J} \), e.g., the Arruda–Boyce and Yeoh models. For the sake of simplicity, only the latter case is considered in this work, the more complicated case is referred to Chen et al. (2022) for reference. Under this circumstance, with \( W \) depending on \( \mathbf{I}_1, \mathbf{J} \), \( \beta \) equals 0, and Eq. (3.5) can be simplified as:

\[
\gamma = \frac{3}{2} \sigma_e^2.
\]

\( (3.6) \)

Once the material coefficients \( \gamma \) is determined, the deviatoric part of the Cauchy stress can be accurately calculated by Eq. (3.3b).

**Remark 1** Since the present work focuses on developing a data-driven topology optimization framework for continuum structures, the material is assumed to be isotropic and hyperelastic to simplify the data-driven analysis algorithm and sensitivity analysis. For materials with more complex mechanical behavior, e.g., elastoplasticity, the data-driven analysis algorithms can be found in recent literatures (Tang et al. 2020, 2021).

### 3.1.2 Database construction

In this work, all the experimental data used are generated by numerical experiments of finite element analysis (FEA). Unless otherwise specified, the analytic-function based constitutive model referred to in this work is the Arruda–Boyce model, which is expressed as:

\[
W = \mu \sum_{i=1}^{5} \frac{C_i}{2^i - 2} \left( \mathbf{I}_1^i - 3^i \right) + \frac{1}{D_1} \left( J^2 - \frac{1}{2} \ln J \right),
\]

\( (3.7) \)

where \( C_1 = \frac{1}{2} C_2 = \frac{1}{20} C_3 = \frac{11}{1050}, C_4 = \frac{19}{7000} \) and \( C_5 = \frac{519}{673750} \) are constant coefficients, the symbols \( \mu = 0.98765 \), \( \lambda = 7 \) and \( D_1 = 0.1 \) are material parameters (Chen et al. 2022). Unless otherwise stated, all quantities in this work are dimensionless.

Uniaxial tension, uniaxial compression, equi-biaxial tension and equi-biaxial compression experiments are numerically performed on a \( 1 \times 1 \times 1 \) unit cubic specimen with the maximum deformation factor illustrated in Fig. 2. Then, based on the equations listed in Fig. 2, totally 5000 data points are sampled uniformly throughout the loading process of each numerical experimental test. The corresponding values of \( \mathbf{b}_e \) and \( \gamma \) of each test are stored in the data sets \( \mathcal{S}_{\text{UT}} = \left\{ (\mathbf{b}_{e, \text{UT}}, \gamma_{\text{UT}})_{i=1,\ldots,5000} \right\} \), \( \mathcal{S}_{\text{UC}} = \left\{ (\mathbf{b}_{e, \text{UC}}, \gamma_{\text{UC}})_{i=1,\ldots,5000} \right\} \), \( \mathcal{S}_{\text{ET}} = \left\{ (\mathbf{b}_{e, \text{ET}}, \gamma_{\text{ET}})_{i=1,\ldots,5000} \right\} \), \( \mathcal{S}_{\text{EC}} = \left\{ (\mathbf{b}_{e, \text{EC}}, \gamma_{\text{EC}})_{i=1,\ldots,5000} \right\} \), respectively, where UT, UC, ET, and EC indicate uniaxial tension, uniaxial compression, equi-biaxial tension, and equi-biaxial compression tests, respectively. Since the values of \( \mathbf{J} \) and \( \sigma_m \) are independent about the loading method, here we combine the data set of the uniaxial tension and equi-biaxial compression tests as \( \mathcal{S} = \left\{ (\mathbf{J}, \sigma_m)_{i=1,\ldots,10000} \right\} \) for a larger deformation range.

**Remark 2** In the loading process of the real experiments, the reaction force \( \mathbf{RF} \) and the displacement \( \mathbf{u} \) of the specimen can be directly measured, and then the 1st Piola–Kirchhoff stress tensor \( \mathbf{P} \) and the deformation gradient \( \mathbf{F} \) can be calculated based on them. As a result, the Cauchy stress \( \mathbf{\sigma} \) in the current configuration is available from \( \mathbf{P} \) and \( \mathbf{F} \). Finally, the quantities used in the data-driven structural analysis algorithm can be given according to the equations in Fig. 2.
### 3.1.3 An artificial neural network-based stress update strategy

Since the data obtained by numerical experiments are discrete, smooth fitting processing is required to ensure the stability and robustness of the structural analysis and sensitivity analysis. Generally, fitting methods such as linear regression, polynomial regression, support vector regression, and artificial neural network (ANN) are often used to process discrete data. Thanks to the flexibility and strong generalization capabilities, five ANNs with the structure shown in Fig. 3 are adopted in this work. The inputs of the five ANNs are $b_{UT}$, $b_{UC}$, $b_{ET}$, $b_{EC}$ and $J$, and their corresponding outputs are $\gamma_{UT}$, $\gamma_{UC}$, $\gamma_{ET}$, $\gamma_{EC}$ and $\sigma_m$, respectively. In addition, in order to demonstrate the robustness of DDSA to data noise, 5% Gaussian random noise is added to each group of experimental data.

The neural network models are trained with the help of Neural Net Fitting toolbox in the Matlab 2014b. Before training these networks, all data sets are normalized within the interval of [-1, 1] and 70%, 15% and 15% of the data sets are randomly selected as the training set, validation set and test set, respectively. The optimizer’s learning rate and maximum epochs are set as 0.01 and 1000, respectively. In addition, the loss function of all networks is the mean square error $MSE = \frac{1}{DN} \sum_{i=1}^{DN} (y_i - \hat{y}_i)^2$, where $DN$ is the total number of data, $y_i$ is the true value, $\hat{y}_i$ is the predicted value, and the Levenberg–Marquardt algorithm is used to minimize the loss function. The fitting results of the ideal data and the data with noise are shown in Figs. 4 and 5, which illustrate that those ANNs achieve perfect smooth fitting even for the data with noise. For conciseness, only the MSE of the training set, validation set, and test set of the data set $S_{UT}$ are given, as shown in Fig. 6, which are $4.94 \times 10^{-9}$, $5.96 \times 10^{-9}$, and $5.02 \times 10^{-9}$, respectively. Furthermore, the MSEs on the test sets of data sets $S_{UC}$, $S_{ET}$, $S_{EC}$ and $S$ are $8.58 \times 10^{-10}$, $3.05 \times 10^{-10}$, $5.00 \times 10^{-9}$ and $1.76 \times 10^{-10}$, respectively. To further quantify the deviation between the predicted and true values, the mean absolute error $MAE = \frac{1}{DN} \sum_{i=1}^{DN} |y_i - \hat{y}_i|$ is also listed in Fig. 4.

Remark 3 The data-driven structural analysis method in this work, i.e., prediction of complex three-dimensional stress states from uniaxial and equi-biaxial experimental data, is derived from the strain energy density function.
of hyperelastic materials, which ensures the physical feasibility of the surrogated constitutive law (Tang et al. 2019; Chen et al. 2022). In the present work, we adopt the neural network models to interpolate an implicit relation of the uniaxial and equi-biaxial experimental data for subsequent structural analysis.

**Remark 4** In principle, many regression models could be applied for the 1D fitting problem of the data-driven analysis algorithm. We compared the performance of ANN (as shown in Fig. 3) and polynomials of the Curve Fitting toolbox of Matlab 2014b on the data set of uniaxial tension experiment, and found that ANN model does have a better performance. More details please refer to Appendix C.

As we all know, in displacement-driven finite element analysis, $J$ and $b_e$ at any material point can be easily obtained by the displacement vector $U$. Therefore, combining $J$ and the corresponding trained ANN, the spherical part $\sigma_m$ of the Cauchy stress can be uniquely determined. According to the trained ANNs, nevertheless, the $b_e$ of a material point corresponds to the four material parameters $\gamma^{UT}$, $\gamma^{UC}$, $\gamma^{ET}$, and $\gamma^{EC}$. Actually, the material parameter $\gamma$ is undoubtedly dependent on the stress state of the material point, which can be judged by the so-called the stress triaxiality introduced in Chen et al. (2022):
When the material point is in uniaxial tension and uniaxial compression states, the corresponding stress triaxiality is $\frac{1}{3}$ and $-\frac{1}{3}$, respectively; and when it is in equi-biaxial tension and equi-biaxial compression states, the corresponding stress triaxiality is $\frac{2}{3}$ and $-\frac{2}{3}$, respectively. Furthermore, we assume that the variation of $\sigma_e$ between the equivalent stress $\sigma_e^{UT}$ of uniaxial tension and the equivalent stress $\sigma_e^{ET}$ of equi-biaxial tension is linear. Then the value of $\sigma_e$ can be calculated as:

$$T = \frac{\sigma_m}{\sigma_e}. \tag{3.8}$$

Substituting Eq. (3.9) into Eq. (3.6), the material coefficient $\gamma$ can be written as:

$$\gamma = (1 - m)\gamma^{UT} + m\gamma^{ET}. \tag{3.10}$$

For the compression states of a material point, in the same way, the material coefficient can be obtained as:
Based on the above discussion, the determination of the material coefficient $\gamma$ can be summarized as:

$$\gamma = (1 - m)\gamma^UC + m\gamma^EC.$$  \hspace{1cm} (3.11)

Based on the above discussion, the determination of the material coefficient $\gamma$ can be summarized as:

$$\gamma = \begin{cases} 
\gamma^EC, & \text{if } T \leq -\frac{2}{3}, \\
(1 - m)\gamma^UC + m\gamma^EC, & \text{if } -\frac{2}{3} < T < -\frac{1}{3}, \\
\gamma^UC, & \text{if } -\frac{1}{3} \leq T < 0, \\
\gamma^UT, & \text{if } 0 \leq T \leq \frac{1}{3}, \\
(1 - m)\gamma^UT + m\gamma^ET, & \text{if } \frac{1}{3} < T < \frac{2}{3}, \\
\gamma^ET, & \text{if } T \geq \frac{2}{3}. 
\end{cases}$$  \hspace{1cm} (3.12)

Once the material coefficient $\gamma$ is given by Eq. (3.12), the Cauchy stress of the material point can be updated as:

$$\sigma = \gamma \sigma \text{dev}(h) + \sigma_m I.$$  \hspace{1cm} (3.13)

In the total Lagrangian formulation, the balance equation of the discrete form can be rewritten as:

$$R(U) = f^{\text{int}} - f^{\text{ext}} = \sum_{e=1}^{ne} L_e^T f_e^{\text{int}} - \sum_{e=1}^{ne} L_e^T f_e^{\text{ext}} = 0.$$  \hspace{1cm} (3.14)

where the internal force vector $f^{\text{int}} = \int_{\Omega} \text{B}^T (\sigma \cdot F^-) \text{d}V$ and it can be calculated by combining Eq. (3.13). Then the analysis result can be obtained by the above-mentioned Newton–Raphson method. It is worth mentioning that the tangent stiffness matrix $K_T(U)$ used in the iteration process is updated by the finite difference method.

### 3.2 Numerical verification of the improved DDSA algorithm

As shown in Fig. 7, a cantilever beam structure with a size of $40 \times 5 \times 10$ is fixed on the left and discretized by $80 \times 10 \times 20$ eight-node hexahedral elements. Uniform vertical downward loads are applied at all the nodes located at the lower edge of the right face for three cases with increasing amplitudes, i.e., $F = 0.03$, $F = 0.05$, $F = 0.07$, respectively. Based on the reference Arruda–Boyce model mentioned above and the constructed database, the analysis results of the three cases are shown in Fig. 8, which includes the Z-direction displacement contour, the maximum displacement of Z-direction and the structural compliance. Furthermore, for a clearer comparison, the relative errors of the results of the DDSA algorithm and their references are listed in Table 1 (all smaller than 2.5%). It can be found that no matter whether noise exists or nor, the DDSA algorithm can accurately obtain the analysis results with very small errors. This example illustrates the effectiveness of the proposed DDSA algorithm and its high robustness to noise.
3.3 Sensitivity analysis and material interpolation model of the DDTO framework

Since the DDSA method is under the displacement-driven finite element analysis framework, the problem formulation of DDTO for three-dimensional hyperelastic continuum structures under finite deformation is the same in form as Eq. (2.3), which can be formulated as:

\[
\begin{align*}
\text{Find } & \quad \mathbf{D} = \left( \left( \mathbf{D}^1 \right)^T, \ldots, \left( \mathbf{D}^n \right)^T, \ldots, \left( \mathbf{D}^{m'} \right)^T \right)^T, 0_u \left( \mathbf{D}; 0x \right), \\
\text{Minimize } & \quad I(\mathbf{D}, 0_u) = \int_\Omega \mathbf{H}^u \left( \chi \left( \mathbf{D}; 0x \right) \right) 0f \cdot 0_u 0d^0 \mathbf{V} + \int_{\partial \Omega} 0_t \cdot 0_u 0d^0 \mathbf{S}, \\
\text{S. t. } & \quad \int_\Omega \mathbf{H}^\delta \left( \chi \left( \mathbf{D}; 0x \right) \right) \mathbf{F} \cdot 0d^0 \mathbf{V} = 0_u \left( \mathbf{D}^{m'} \right)^T \mathbf{P}^{0_u} \mathbf{d}^0 \mathbf{V} + \int_{\partial \Omega} 0_t \cdot 0_u 0d^0 \mathbf{S}, \forall 0_u \mathbf{d}^0 \mathbf{V} \in \mathbf{U}^0_{\text{ad}},
\end{align*}
\]

where \( \mathbf{P} = \mathcal{F}(\mathbf{F}, \mathbf{J}; \mathbf{NN}_1, \mathbf{NN}_2, \mathbf{NN}_3, \mathbf{NN}_4, \mathbf{NN}_5) \),

\[
\int_{\partial \Omega} \mathbf{H}^u \left( \chi \left( \mathbf{D}; 0x \right) \right) d^0 \mathbf{V} \leq 0^0 \mathbf{V},
\]

\[
P = \mathcal{F}(\mathbf{F}, \mathbf{J}; \mathbf{NN}_1, \mathbf{NN}_2, \mathbf{NN}_3, \mathbf{NN}_4, \mathbf{NN}_5),
\]

\[
\int_{\partial \Omega} \mathbf{H}^\delta \left( \chi \left( \mathbf{D}; 0x \right) \right) \mathbf{F} \cdot 0d^0 \mathbf{V} = 0_u \left( \mathbf{D}^{m'} \right)^T \mathbf{P}^{0_u} \mathbf{d}^0 \mathbf{V} + \int_{\partial \Omega} 0_t \cdot 0_u 0d^0 \mathbf{S}, \forall 0_u \mathbf{d}^0 \mathbf{V} \in \mathbf{U}^0_{\text{ad}}.
\]

Table 1 The relative errors of the results of the DDSA and their reference values

| Force | \( U_{\text{max}}^\text{(without noise)} \) (%) | \( U_{\text{max}}^\text{(with noise)} \) (%) | Compliance \( \text{(without noise)} \) (%) | Compliance \( \text{(with noise)} \) (%) |
|-------|---------------------------------|---------------------------------|---------------------------------|---------------------------------|
| 0.03  | 1.60                            | 1.78                            | 1.91                            | 2.08                            |
| 0.05  | 1.67                            | 1.78                            | 1.95                            | 2.03                            |
| 0.07  | 1.75                            | 1.83                            | 1.92                            | 1.94                            |

\[
\mathbf{D} \in \mathbf{U}_P,
\]

\[
0_u = 0, \text{ on } \partial \Omega
\]

\[
(3.15)
\]

where \( \mathbf{NN}_1, \mathbf{NN}_2, \mathbf{NN}_3, \mathbf{NN}_4, \text{ and } \mathbf{NN}_5 \) are the network parameters corresponding to the five ANNs trained in sub-Sect. 3.1.3, respectively. It is worth noting that for any material point in the structure, the 1st Piola–Kirchhoff stress tensor \( \mathbf{P} \) is no longer determined by the analytic-function based \( \mathbf{W} \), but is given by combining the constructed database and the stress update strategy in the DDTO framework.

The solution strategies of DDTO framework, such as sensitivity analysis and numerical stabilization technique, can perfectly transplant their counterparts CMTO uses, e.g., the adjoint sensitivity analysis method and the redundant degrees of freedom removal technique in sub-Sect. 2.3. As a result, the sensitivity of the objective function in DDTO framework is the same in form as Eq. (2.11). As compared to the sensitivity analysis of CMTO, the only difference in sensitivity of the objective function in DDTO method is that the nodal internal force vector \( f^0_{\text{int}} \) of the \( e \) th element is calculated by the stress update strategy and the tangent stiffness matrix \( \mathbf{K}_E \left( \mathbf{D}, \mathbf{U}_E \right) \) used in Eq. (2.12) is given by the finite difference method.

Additionally, according to Eqs. (2.5), (3.2), (3.3a) and (3.3b), the material interpolation model of DDTO can be expressed as:
where $\sigma_e$ is the Cauchy stress of the $e$th element, and $\sigma_0$ is the Cauchy stress obtained by combining the constructed database and the stress update strategy (in Sect. 3.1.2 and 3.1.3). The flowchart of the proposed DDTO framework is shown in Fig. 9.

\[
\sigma_e = \sum_{i=1}^{mn} H_e^a(\chi^a(D;0,x)^c) \left( \gamma \text{dev}(b) + \sigma_m I \right) \\
= \sum_{i=1}^{mn} H_e^a(\chi^a(D;0,x)^c) \sigma_0, 
\]

(3.16)

where $\sigma_e$ is the Cauchy stress of the $e$th element, and $\sigma_0$ is the Cauchy stress obtained by combining the constructed database and the stress update strategy (in Sect. 3.1.2 and 3.1.3). The flowchart of the proposed DDTO framework is shown in Fig. 9.

\[
V_{\text{var}} = \left| \frac{V(D)}{V_D} - \frac{0V}{V_D} \right|,
\]

\[
obj_{\text{var}} = \begin{cases} 1.0, & \text{if } \text{iter} < 5, \\
\frac{\sum_{\text{iter}=4}^{\text{iter}} |\text{obj} - \text{obj}_{\text{iter}}|}{5\text{obj}_{\text{iter}}}, & \text{otherwise}, 
\end{cases}
\]

(4.1)

### 4 Numerical examples

In this section, several examples are studied to demonstrate the effectiveness and stability of the proposed DDTO framework for three-dimensional continuum structures under finite deformation. The experimental data and the analytic-function based constitutive model used in the numerical examples are given in sub-Sect. 3.1.2 unless otherwise stated. The optimization problems are solved by the well-known Method of Moving Asymptotes (MMA) (Svanberg 1987) and terminated by the convergence criterion of $V_{\text{var}} < 10^{-3}$ and $\text{obj}_{\text{var}} < 10^{-3}$, where $V_{\text{var}}$, $\text{obj}_{\text{var}}$ are defined as
where $V(D)$ is the volume of the current design, $\text{iter}$ is the number of current iteration, $\text{obj}^i$ is the objective function value at the $i$th iteration.

4.1 The three-dimensional cantilever beam example

In order to verify the effectiveness of the 3D-MMV based explicit topology optimization algorithm for continuum structures with an analytic-function based constitutive model (i.e., the CMTO method), the cantilever beam example described by Sect. 3.2 and Fig. 7 is investigated first. The amplitudes of the external nodal loads are set as $F = 0.02$, $F = 0.025$, $F = 0.04$, $F = 0.06$, respectively. Setting the initial design shown in Fig. 10 and the upper bound of the volume fraction of the solid material as 0.5, the optimized results of the four loading cases are shown in Table 2, respectively. According to the optimized results in Table 2, significant differences are found between the optimized structures of the four cases, which are consistent with the results in literature (Chen et al. 2017). Furthermore, the stable iteration history curve of the case with $F = 0.06$ is presented in Fig. 11.

4.2 The three-dimensional two-ends clamped beam example

As shown in Fig. 12, the design domain with a size of $60 \times 5 \times 10$ is discretized by $120 \times 10 \times 20$ eight-node hexahedra elements. Both ends of the design domain are fixed and the downward nodal loads of three cases, i.e., $F = 0.1$, $F = 0.3$, $F = 0.6$, respectively, are imposed on all the nodes located at the center line of the bottom of the design domain. The initial design shown in Fig. 13 contains 64 voids with 4160 design variables and the upper bound of the volume fraction of the solid material is set as 0.5. This example is

![Fig. 10 The initial design for the three-dimensional cantilever beam](image)

![Table 2 The optimized results of the four cases solved by the CMTO method](table)

![Fig. 11 The iterative history curve of $F = 0.06$ of the cantilever beam example](image)
solved both by the proposed CMTO method and the DDTO method with the dataset shown in Fig. 4.

The optimized results corresponding to the three cases and the iterative curves of $F = 0.1$ are shown in Table 3 and Fig. 14, respectively. It can be found that, both of the proposed algorithms converge stably. Furthermore, as illustrated by Table 3, both the optimized structures of DDTO method and CMTO method have significant topology changes as the variation of the amplitude of the external load, which is caused by the consideration of the material and geometrical nonlinearities. Besides, only small differences are observed between the optimized structures obtained by the DDTO and CMTO methods, and the relative errors of the objective function values for the three load cases are all smaller than 3%. These results demonstrate the correctness and validity of the proposed DDTO method.

4.3 The three-dimensional simply supported beam example

This simply supported beam example shown in Fig. 15 is to test the robustness of the proposed DDTO algorithm against data noise. The size of the design domain is $60 \times 5 \times 10$ and $120 \times 10 \times 20$ uniform eight-node hexahedra elements are used for discretizing the design domain. The vertical downward nodal loads with magnitudes of $F = 0.1$ are imposed on all the nodes located at the center line of the bottom of the design domain. The initial design is the same as in example 4.2, as shown in Fig. 13. The upper bound of the volume fraction of the base material is set as 0.5. Under the conditions mentioned above, this example is solved by the DDTO algorithm with noisy data set (as shown in Fig. 5), the DDTO algorithm with ideal data set (as shown in Fig. 4) and the CMTO algorithm, respectively. The corresponding optimized structures, compliance values and their relative errors are shown in Table 4. Those optimized designs are very close and the relative error of the compliance values of the DDTO designs are smaller than 3% as compared to the results obtained by the CMTO method, which validates that the proposed DDTO framework is also robust to data noise.

Since the data obtained in the real experiment could be sparse and accompanied by noise, the amount of data in the above data set is reduced to 50. Both ideal and noisy data sets (2% Gaussian random noise) are evaluated. Using the neural network model shown in Fig. 3, the corresponding fitting results are shown in Fig. 16 and Fig. 17, respectively. Furthermore, based on those data sets, the optimized simply supported beams obtained by the DDTO algorithm are shown in Table 4. Interestingly, the design results of the sparse data sets with and without noise are still close to the corresponding optimized designs of the CMTO method, and the relative errors of compliance values are smaller than 3%. This demonstrates that the proposed DDTO framework is also effective for sparse data set with moderate noise.

4.4 The three-dimensional torsion beam example

Finally, the three-dimensional torsion beam is discussed to verify the effectiveness of the proposed DDTO algorithm for optimized structures with complex stress states. As illustrated in Fig. 18a, a $12 \times 4 \times 4$ beam is fixed at the left-hand side and the nodal loads of magnitude 0.02 are applied at all the nodes located at the four yellow lines on the right face BAC, resulting in a counter-clockwise torque (see Fig. 18b for reference). The left and right sides (both have a dimension of $0.4 \times 4 \times 4$) are defined as non-designable solid domain. For the DDSA, $60 \times 20 \times 20$ eight-node hexahedra elements are created. The initial design shown in Fig. 19 contains 88 voids with 5720 design variables, and the upper bounds of the volume fraction of the material are set as $0 \bar{V} = 0.5$ and $0 \bar{V} = 0.3$, respectively. This example is solved by the proposed DDTO method with ideal data set (as shown in Fig. 4) and the CMTO algorithm as well. The optimized results and the iterative history curves of $0 \bar{V} = 0.5$ are shown in Table 5, Table 6 and Fig. 20, respectively. As shown in Tables 5 and 6, both algorithms obtain a thin-walled cylindrical structure, and the cylindrical wall becomes thinner as the upper bound of the volume fraction of the base material becomes smaller. Furthermore,
Table 3  The optimized results of the three cases solved by the CMTO and DDTO methods

| Framework | Force | Optimized structures | Compliance | Relative error (%) |
|-----------|-------|----------------------|------------|--------------------|
| CMTO      | 0.1   |                      | 2.39       | 2.93               |
| DDTO      | 0.1   |                      | 2.32       |                    |
| CMTO      | 0.3   |                      | 18.42      | 2.88               |
| DDTO      | 0.3   |                      | 17.89      |                    |
| CMTO      | 0.6   |                      | 62.27      | 2.28               |
| DDTO      | 0.6   |                      | 60.85      |                    |

The relative errors of the compliance values are both small for the cases \( \sigma V = 0.5 \) and \( \sigma V = 0.3 \), i.e., 2.94% and 2.17%, respectively, which shows that the proposed DDTO method is also effective despite complex stress states.
Thanks to the adoption of the redundant degrees of freedom removal technique, the DDTO algorithm can not only achieve a stable convergence during the optimization process (see Fig. 20), but also significantly reduce the number of involved DOFs in the nonlinear finite element analysis as shown in Fig. 21. In addition, the optimized structure can be directly constructed by the CAD system as shown in Fig. 22, since the topology of the structure is described by explicit geometric parameters under the proposed DDTO framework.

Appendix A

\[ r(\theta, \varphi) = \|S(u(\theta), v(\varphi))\| = \| \sum_{k=0}^{K} \sum_{l=0}^{L} N_{k,p}(u(\theta))N_{l,q}(v(\varphi))p^{k,l} \|, \]  

where \( N_{k,p}(u)N_{l,q}(v) \) are the B-spline basis functions of \( p \) th and \( q \) th orders, \( K = 14 \) and \( L = 6 \) are the total number of control points in the \( \theta \) and \( \varphi \) directions, respectively. The symbols \( p^{k,l} = \left( p^{k,l}_x, p^{k,l}_y, p^{k,l}_z \right)^T \), \( k = 0, \ldots, K, l = 0, \ldots, L \) are the coordinates of the corresponding control points. In order to avoid self-intersection of the surfaces, the control points are constructed as follows:

5 Concluding remarks

In the present work, a data-driven topology optimization (DDTO) framework for three-dimensional continuum structures under finite deformation is proposed. The advantages of proposed DDTO framework can be summarized as follows: (1) In the DDTO framework, topology optimization of the three-dimensional continuum structure under finite deformation is implemented only by the uniaxial and equi-biaxial experimental data, without using the analytic-function based constitutive models. (2) Since the data-driven analysis method is still under the framework of the finite element method, the solution strategies used in traditional topology optimization method such as sensitivity analysis and redundant degrees of freedom removal technique can be perfectly transplanted to the DDTO framework. (3) Described by a series of NURBS surfaces, the optimized structure has explicit geometry and can be constructed in CAD system directly. Although only minimum end compliance design is considered in the present work, with the assumption of hyperelasticity of the considered material, the DDTO framework can also be extended to topology optimization problems considering the effects of multi-material, stress, frequency, buckling, etc. For materials with more general nonlinear behaviors, e.g., elastoplastic and viscoelastic materials, the data-driven topology optimization of the three-dimensional continuum structure still requires further efforts.
where \( r_{k,l} \), \( k = 0, \ldots, K \), \( l = 0, \ldots, L \) is the distance from the control point to the center of the void, \( \theta_k = \frac{2\pi k}{K} \), \( k = 0, \ldots, K \), \( \varphi_l = \frac{\pi l}{L} \), \( l = 0, \ldots, L \). Since the surface is a closed region, it is also required that

\[
P_{x}^{k,l} = r_{k,l}^k \sin(\varphi_l) \cos(\theta_k),
\]

(A.2a)  \( r_{0,l}^0 = r_{K,l}^K, l = 0, \ldots, L, \)

(A.3a)

\[
P_{y}^{k,l} = r_{k,l}^k \sin(\varphi_l) \sin(\theta_k),
\]

(A.2b)  \( r_{k,0}^{k,0} = r_{k,0}^{k,0}, k = 1, \ldots, K, \)

(A.3b)

\[
P_{z}^{k,l} = r_{k,l}^k \cos(\varphi_l),
\]

(A.2c)  \( r_{k,L}^{k,L} = r_{k,L}^{k,L}, k = 1, \ldots, K. \)

(A.3c)

**Appendix B**

\[
\frac{\partial X^i}{\partial D} = \sum_{i=1}^{m} \frac{\partial X^i}{\partial D^i(D';x)} \frac{\partial X^i(D';x)}{\partial D} = \sum_{i=1}^{m} \sum_{j=1}^{m} e^{-i\beta(D';x)} \frac{\partial X^i(D';x)}{\partial D}.
\]

(B.1)
In Eq. (2.11), the derivative of $\chi^i(D'x)$ with respect to each design variable can be calculated as follows:

$$\frac{\partial \chi^i(D'x)}{\partial C^i_x} = \frac{C^i_x}{\sqrt{(x - C^i_x)^2 + (y - C^i_y)^2 + (z - C^i_z)^2}},$$

(B.2)

$$\frac{\partial \chi^i(D'x)}{\partial C^i_y} = \frac{C^i_y}{\sqrt{(x - C^i_x)^2 + (y - C^i_y)^2 + (z - C^i_z)^2}},$$

(B.3)

$$\frac{\partial \chi^i(D'x)}{\partial C^i_z} = \frac{C^i_z}{\sqrt{(x - C^i_x)^2 + (y - C^i_y)^2 + (z - C^i_z)^2}},$$

(B.4)

$$\frac{\partial \chi^i(D'x)}{\partial r_k^l} = \frac{1}{r(\theta, \varphi)} \left[ S_x(\theta, \varphi) \frac{\partial S_y(\theta, \varphi)}{\partial r_k^l} + S_y(\theta, \varphi) \frac{\partial S_z(\theta, \varphi)}{\partial r_k^l} \right].$$

(B.5)
where
\[
\frac{\partial S_x(\theta, \varphi)}{\partial r_{k,l}} = \sum_{n=1}^{K} \sum_{m=1}^{L} N_{n,p}(u(\theta))N_{m,q}
\]

\[
(n(\varphi)) \frac{\partial P_{m,m}^{n,m}}{\partial r_{k,l}}, n = 0, \ldots, K, m = 0, \ldots, L, \text{ (B.6)}
\]

\[
\frac{\partial S_y(\theta, \varphi)}{\partial r_{k,l}} = \sum_{n=1}^{K} \sum_{m=1}^{L} N_{n,p}(u(\theta))N_{m,q}
\]

\[
(n(\varphi)) \frac{\partial P_{m,m}^{n,m}}{\partial r_{k,l}}, n = 0, \ldots, K, m = 0, \ldots, L, \text{ (B.7)}
\]
Fig. 18 The three-dimensional torsion beam example, a the design domain with left-hand side fixed, b uniform loads are applied to the four yellow lines on the face BAC, resulting in a counter-clockwise torque.

Table 5 The optimized results of the three-dimensional torsion beam of $\sqrt{V} = 0.5$

|           | CMTO | DDTO |
|-----------|------|------|
| Optimized structures | ![CMTO](image) | ![DDTO](image) |
| Cross section | ![CMTO](image) | ![DDTO](image) |
| Compliance   | 0.34  | 0.33  |
| Relative error | —     | 2.94% |
Table 6  The optimized results of the three-dimensional torsion beam of $V = 0.3$

| CMTO | DDTO |
|------|------|
| Optimized structures | |
| Cross section | |
| Compliance | 0.46 | 0.45 |
| Relative error | — | 2.17% |
\[ \frac{\partial P_{x,l}}{\partial r_{k,l}} = \sin(\varphi_j)\cos(\theta_j), \]
\[ \frac{\partial P_{y,l}}{\partial r_{k,l}} = \sin(\varphi_j)\sin(\theta_j), \]
\[ \frac{\partial P_{z,l}}{\partial r_{k,l}} = \cos(\varphi_j), \] (B.9)
otherwise, \( \partial P_{x,m}/\partial r_{k,l} = 0, \partial P_{y,m}/\partial r_{k,l} = 0, \partial P_{z,m}/\partial r_{k,l} = 0. \)

\section*{Appendix C}

See Tables 7 and 8.

\begin{table}[h]
\centering
\caption{The mean square errors of ANN and polynomials in fitting different numbers of ideal data of the uniaxial tension experiment.} 
\begin{tabular}{|c|c|c|c|}
\hline
Number of data & ANN & Polynomial (Degree: 3) & Polynomial (Degree: 8) \\
\hline
50 & 2.29 \times 10^{-9} & 1.60 \times 10^{-3} & 4.48 \times 10^{-5} \\
500 & 1.87 \times 10^{-9} & 1.50 \times 10^{-3} & 4.54 \times 10^{-5} \\
5000 & 1.87 \times 10^{-9} & 1.50 \times 10^{-3} & 4.54 \times 10^{-5} \\
\hline
\end{tabular}
\end{table}

\begin{table}[h]
\centering
\caption{The mean square errors of ANN and polynomials in fitting different numbers of noisy data of the uniaxial tension experiment.} 
\begin{tabular}{|c|c|c|c|}
\hline
Number of data & ANN & Polynomial (Degree: 3) & Polynomial (Degree: 8) \\
\hline
50 & 3.52 \times 10^{-3} & 1.71 \times 10^{-2} & 1.79 \times 10^{-2} \\
500 & 3.52 \times 10^{-3} & 1.55 \times 10^{-2} & 1.55 \times 10^{-2} \\
5000 & 4.52 \times 10^{-3} & 1.62 \times 10^{-2} & 1.61 \times 10^{-2} \\
\hline
\end{tabular}
\end{table}
As shown in the above two tables, the ANN performs better on both ideal and noisy data sets, and ANN is adopted as the fitting tool in this work.

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Declarations

Conflict of interest The authors declare they have no conflict of interest.

Replication of results Code and data for replication can be provided up on request.

References

Allaire G, Jouve F, Toader AM (2004) Structural optimization using sensitivity analysis and a level-set method. J Comput Phys 194:363–393

Bendsøe MP (1989) Optimal shape design as a material distribution problem. Struct Optim 1:193–202

Bendsøe MP, Kikuchi N (1988) Generating optimal topologies in structural design using a homogenization method. Comput Methods Appl Mech Eng 71:197–224

Bonatti C, Mohr D (2022) On the importance of self-consistency in recurrent neural network models representing elasto-plastic solids. J Mech Phys Solids 158:104697

Buhl T, Pedersen CBW, Sigmund O (2000) Stiffness design of geometries (MMC) method for three-dimensional topology optimization. Struct Multidisc Optim 59:1895–1913

Du Z, Cui T, Liu C, Zhang W, Guo Y, Guo X (2022) An efficient and easy-to-extract Matlab code of the Moving Morphable Component (MMC) method for three-dimensional topology optimization. Struct Multidisc Optim 65:158

Guo X, Zhang WS, Zhong WL (2014) Doing topology optimization explicitly and geometrically—a new moving morphable components based framework. J Appl Mech 81:081009

Guo X, Du Z, Liu C, Tang S (2021) A new uncertainty analysis-based framework for data-driven computational mechanics. J Appl Mech 88:111003

Ha SH, Cho S (2008) Level set based topological shape optimization of geometrically nonlinear structures using unstructured mesh. Comput Struct 86:1447–1455

He Q, Chen JS (2020) A physics-constrained data-driven approach based on locally convex reconstruction for noisy database. Comput Methods Appl Mech Eng 363:112791

Huang J, Xu S, Ma Y, Liu J (2022) A topology optimization method for hyperelastic porous structures subject to large deformation. Int J Mech Mater Des 18:289–308

Ibañez R, Borzacchiello D, Agudo JV, Abisset-Chavanne E, Cueto E, Ladeveze P, Chinesta F (2017) Data-driven nonlinear elasticity: constitutive manifold construction and problem discretization. Comput Mech 60:813–826

Ibañez R, Abisset-Chavanne E, Agudo JV, Gonzalez D, Cueto E, Chinesta F (2018) A manifold learning approach to data-driven computational elasticity and inelasticity. Arch Comput Methods Eng 25:47–57

Kanno Y (2018) Simple heuristic for data-driven computational elasticity with material data involving noise and outliers: a local robust regression approach. Jpn J Ind Appl Math 35:1085–1101

Kirschdoerfer T, Ortiz M (2016) Data-driven computational mechanics. Comput Methods Appl Mech Eng 304:81–101

Lahuerta RD, Simões ET, Campello EM, Pimenta PM, Silva EC (2013) Towards the stabilization of the low density elements in topology optimization with large deformation. Comput Mech 52:779–797

Luo Y, Wang MY, Kang Z (2015) Topology optimization of geometrically nonlinear structures based on an additive hyperelasticity technique. Comput Methods Appl Mech Eng 286:422–441

Masi F, Stefanou I, Vannucci P, Maffi-Berthier V (2021) Thermodynamics-based artificial neural networks for constitutive modeling. J Mech Phys Solids 147:104277

Silva ALF, Salas RA, Silva ECN, Reddy JN (2020) Topology optimization of fibers orientation in hyperelastic composite material. Comput Struct 231:111488

Svanberg K (1987) The method of moving asymptotes—a new method for structural optimization. Int J Numer Methods Eng 24:359–373

Tang S, Zhang G, Yang H, Li Y, Liu WK, Guo X (2019) MAP 123: A data-driven approach to use 1D data for 3D nonlinear elastic materials modeling. Comput Methods Appl Mech Eng 357:112587

Tang S, Li Y, Qiu H, Yang H, Saha S, Momjundar S, Liu WK, Guo X (2020) MAP123-EP: a mechanistic-based data-driven approach for numerical elastoplastic analysis. Comput Methods Appl Mech Eng 364:112955

Tang S, Yang H, Qiu H, Fleming M, Liu WK, Guo X (2021) MAP123-EPF: a mechanistic-based data-driven approach for numerical elastoplastic modeling at finite strain. Comput Methods Appl Mech Eng 373:113484

van Dijk NP, Langelaar M, van Keulen F (2014) Element deformation scaling for robust geometrically nonlinear analyses in topology optimization. Struct Multidisc Optim 50:537–560

Wang MY, Wang XM, Guo DM (2003) A level set method for structural topology optimization. Comput Methods Appl Mech Eng 192:227–246

Wang F, Lazarov BS, Sigmund O, Jensen JS (2014) Interpolation scheme for fictitious domain techniques and topology optimization of finite strain elastic problems. Comput Methods Appl Mech Engrg 276:453–472
Xia Q, Shi T (2016) Stiffness optimization of geometrically nonlinear structures and the level set based solution. Int J Simul Multisci Des Optim 7:A3
Xie YM, Steven GP (1993) A simple evolutionary procedure for structural optimization. Comput Struct 49:885–896
Xue R, Liu C, Zhang W, Zhu Y, Tang S, Du Z, Guo X (2019) Explicit structural topology optimization under finite deformation via Moving Morphable Void (MMV) approach. Comput Methods Appl Mech Eng 344:798–818
Yoon GH, Kim YY (2005) Element connectivity parameterization for topology optimization of geometrically nonlinear structures. Int J Solids Struct 42:1983–2009
Yoon GH, Kim YY (2007) Topology optimization of material-nonlinear continuum structures by the element connectivity parameterization. Int J Numer Methods Engrg 69:2196–2218
Zhang XS, Chi H (2020) Efficient multi-material continuum topology optimization considering hyperelasticity: achieving local feature control through regional constraints. Mech Res Commun 105:103494
Zhang W, Chen J, Zhu X, Zhou J, Xue D, Lei X, Guo X (2017) Explicit three dimensional topology optimization via Moving Morphable Void (MMV) approach. Comput Methods Appl Mech Engrg 322:590–614
Zhang Z, Zhao Y, Du B, Yao W (2020a) Topology optimization of hyperelastic structures using a modified evolutionary topology optimization method. Struct Multidisc Optim 62:3071–3088
Zhang XS, Chi H, Paulino GH (2020b) Adaptive multi-material topology optimization with hyperelastic materials under large deformations: a virtual element approach. Comput Methods Appl Mech Eng 370:112976
Zhou M, Rozvany GIN (1991) The COC algorithm, Part II: topological, geometrical and generalized shape optimization. Comput Methods Appl Mech Eng 89(1–3):309–336
Zhou Y, Zhan H, Zhang W, Zhu J, Bai J, Wang Q, Gu Y (2020) A new data-driven topology optimization framework for structural optimization. Comput Struct 239:106310

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