Suppressing Gray-Scale Elements in Topology Optimization of Continua Using Modified Optimality Criterion Methods

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Abstract: This study proposes a new topology optimization method for continuum structures, which includes modified heuristic optimality criteria in conjunction with the SIMP scheme to suppress gray-scale elements occurred in topology optimization of continua through smoothed Heaviside function. In the process of numerical implementation, the gray scale elements are suppressed to approach the binary bounds of 0 or 1 by utilizing the proposed approach and the corresponding convergence criterion. Two typical numerical examples are used to demonstrate the effectiveness of the proposed method in suppressing the gray-scale elements with intermediate densities, as well as the efficiency of this method in the numerical procedure.

Keywords: Topology optimization; Continuum structure; Optimality Criterion; Gray-scale elements; SIMP method.

1 Introduction

Since one of the pioneering works in the area of topology optimization for continuum structures using the homogenization method by Bendsøe and Kikuchi (1988), topology optimization has become one of the most important but challenging techniques in the area of structural optimization of topology, shape and size. Topology optimization [Bendsøe and Sigmund (2003)] is essentially a numerical procedure to iteratively distribute a given amount of material in the design space to search its best configuration to bear loads effectively, so as to determine the best material layout by optimizing the prescribed objective function subject to specific con-

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straint(s). The design of topological optimization has drawn much consideration over the past two decades, and many different methods have been developed for a number of engineering applications, such as [Maute and Frangopol (2003); Luo, Yang and Chen (2006); Dühring, Jensen and Sigmund (2008); Kang and Tong (2008); Luo, Tong and Ma (2009)]. The typical methods for topology optimization include the homogenization [Bendsøe and Kikuchi (1988)], SIMP (solid isotropic microstructures with penalization) [Zhou and Rozvany (1991); Bendsøe and Sigmund (1999)], and level set-based methods [Wang, Wang and Guo (2003); Allaire, Jouve and Toader (2004)]. With the development of modern computational methods, topology optimization is becoming a more preferred industrial design tool in the stage of conceptual design.

In fact, the topology optimization of continua belongs to a family of integer programming problems with 0 and 1 discrete design variables, to which many gradientbased optimization algorithms cannot be directly applied. To overcome this shortcoming, the original discrete optimization problem can be relaxed to allow the discrete design variables to continuously take intermediate densities from 0 to 1. As an extension of the homogenization method, SIMP is becoming popular because of its conceptual and numerical simplicity. However, an exponential 'power-law' scheme [Bendsøe and Sigmund (1999)] is usually included to penalize the intermediate densities. To ensure a meaningful solution of the relaxed problem close to the original 0 and 1 design, additional schemes, including the sensitivity filter [Sigmund (2001)], density-sensitivity filter [Luo, Chen, Yang, Zhang and Abdel-Malak (2005)] or morphology-based filter [Sigmund (2007)], are included to the problem to avoid numerical instabilities, e.g. checkerboards and mesh-dependences [Diaz and Sigmund (1995); Sigmund and Petersson (1998)].

Although the above mentioned schemes can be used to overcome the typical numerical instabilities, it is common to generate designs involving gray-scale elements, because a portion of material with intermediate densities will appear surrounding structural boundaries. This makes it hard to interpret the final topological design accurately due to the blur boundaries, as an under or over evaluated structural boundary is undesirable. In order to suppress gray-scale elements, there have been a lot of research endeavors with a view to solving this problem. For instance, Xu, Cai and Cheng (2010) proposed a nonlinear filtering method to satisfy the volume constraint and got clear boundary of the topology optimization. Groenwold and Etman (2009) proposed a heuristic criterion method to suppress the gray-scale elements. However, it is difficult to determine the relevant parameters and the iteration procedure is computationally expensive. Some popular filtering schemes, such as [Bourdin (2001); Sigmund (2001); Luo, Chen, Yang, Zhang and Abdel-Malak (2005); Sigmund (2007)], can be applied to eliminate numerical instabilities

including checkerboards. However, most of the above methods cannot be used to effectively suppress the gray-scale elements around the boundary of structures.

To suppress the gray-scale elements, this paper proposed two heuristic Optimality Criterion (OC) formulas based on the Logistic regression analysis function through a regression analysis model to estimate the corresponding parameters, namely, a Modified Optimality Criterion (MOC) method. OC methods have been widely employed in the area of topological optimization due to its advantages [Zhou and Rozvany (1991); Rozvany, Bendsøe and Kirsch (1995)]. In combination with the conventional SIMP model and a special convergence criterion, the MOC method is expected to create better optimal designs in topology optimization. The typical numerical examples are used to showcase the effectiveness of the proposed method, which possesses the advantages to effectively suppress the gray-scale elements, with a fast convergence, and a unified and simple form of iteration formula.

2 Structure topology optimization model

Topology optimization is often formulated as a material distribution problem, in which solid and void phases are indicated by discrete values 1 and 0, respectively. As aforementioned, the discrete model is usually required to be relaxed to make material properties continuously dependent on the local amount of material. SIMP [Zhou and Rozvany (1991); Bendsøe and Sigmund (1999)] has been widely used for synthesizing optimal topology of structures, due to its conceptual simplicity, implementation easiness and computational efficiency. The key procedure of SIMP is to regularize the original optimization problem with 0 and 1 discrete design variables into a relaxed one with design variables ranging from 0 to 1 continuously. In doing so, more efficient gradient-based optimization algorithms can be applied to solve topology optimization problems of structures.

2.1 SIMP interpolation scheme

In SIMP, a density-stiffness interpolation scheme is used to represent the nonlinear dependency between elemental densities and material properties. To recover the original 0 and 1 discrete material distribution, a power-law scheme [Bendsøe and Sigmund (1999)] is usually applied to penalize the intermediate densities to push the intermediate densities towards its binary bounds (0/1). In most engineering applications, the SIMP method can be generally written as

$$E_e(x_e) = x_e^p E_0 \tag{1}$$

$$\rho_e(x_e) = x_e \rho_0 \left(0 \le x_e \le 1 \right) \tag{2}$$

where E_e and E_0 denote the actual and initial Young's Modulus, respectively, p is the penalty factor. ρ_0 is the material's density of solid state, ρ_e is the element material's density, and x_e is the element's relative density. In addition, the design variables ρ_e need to be iteratively updated, and so the Young's Modulus is also reevaluated for the structural analysis of the next iteration.

However, E_0 is a constant value (the relative value is 1.0) in a given topology optimization problem, so Eq. (1) is an exponential function. With the increasing of the penalty factor p, the result value of $E_e(x_e)$ will become better. If the penalty factor p is too big or too small, it will lead to numerical instabilities, including the porous materials, the checkerboard phenomenon, difficulty of convergence and so on. So the penalty factor is an important element in SIMP, which should be taken into consideration for a relative good value in a given problem.



Figure 1: SIMP model with different penalty factors

Fig. 1 shows different shapes of the penalty factor when p is given different values. From the graph, one can see that in SIMP scheme, the penalty factor should not be too small or too big. For example, it will not reach the goal if the value is 1.0. When the penalty factor is 9.0, the result will become worse because of deleting too many high-relative-density elements. In general, p is 3.0 in SIMP scheme.

From Fig. 1, it can be seen that most elements' relative densities are located between 0.4 and 0.9. When the relative density is less than 0.4, Eq. (1) will make the corresponding *Young's Modulus of relative materials* close to 0, which can be solved efficiently. But the penalty curve shows that just a small number of highrelative-density elements (between 0.9-1.0) are pushed to 1.0. In addition, when the relative densities are between 0.4 and 0.9, Eq. (1) will produce many intermediate relative Young's Moduli ranging from 0.08 to 0.72. This phenomenon will produce a great number of porous material elements in the final topology, namely, gray-scale elements.

2.2 Optimization formulation with SIMP

In the SIMP method, the design domain is discretized into a finite element (FE) mesh defined by N_x , which is the set of elements in the *x*-axis ($N_x = \{1, 2, ..., |N_x|\}$) and N_y , which is the set of elements in the *y*-axis ($N_y=\{1, 2, ..., |N_y|\}$). The relative density of every element in the mesh (x_e , $e \in N_x \times N_y$) is considered as a design variable ($0 \le x_e \le 1$). SIMP method assumes that the stiffness matrix of each element depends on the relative density raised to some penalization power, *p*. Thus, the optimization problem for obtaining the minimum compliance can be written as:

$$\begin{cases} \text{Find} : x = (x_1, x_2, x_3, ..., x_N)^{\mathrm{T}} \\ \text{Min} : C(x) = \mathbf{U}^{\mathrm{T}} \mathbf{K} \mathbf{U} = \sum_{e=1}^{N} (x_e)^{p} u_e^{\mathrm{T}} k_0 u_e \\ s.t. : V(x)/V_0 \le f \\ \mathbf{K} \mathbf{U} = \mathbf{F} \end{cases}$$
(3)

where $x = (x_1, x_2, ..., x_N)^T$ is an *N*-dimensional vector of design variables, in which $0 < x_{\min} \le x_e \le x_{\max} \le 1$. C(x) is the mean compliance of the structure, defined by the density vector *x* of design variables x_e ; *K* is the global stiffness matrix, *U* and *F* are the global displacement and force vectors, respectively. $N(N=N_x \times N_y)$ is the number of elements used to discretize the design domain. u_e is the element displacement vector, k_0 is the element stiffness matrix; *f* is the prescribed volume fraction; x_{min} and x_{max} are the lower and upper bounds of the relative densities (non-zero to avoid numerical singularity); V(x) and V_0 is the given material volume and the design domain volume, respectively.

2.3 Numerical instabilities

Checkerboard, mesh-dependences and local minima are the common numerical instabilities in the topology optimization of continuum structures. For example, the checkerboard problem refers to the formation of regions of alternating solid and void elements arranged in a checkerboard-type fashion. Many approaches [Sigmund and Petersson (1998)] have been proposed to handle these problems. For the checkerboard, the widely used methods include higher-order finite elements, filters, nodal-density projection methods and geometric constraints and so on. In particular, the filter method is a simple but effective heuristic method to overcome checkerboards and mesh-dependences. The merit of this method is that it will not add any constraints to the optimization problem, easy to implement in the numerical procedure.

Based on filtering techniques from image processing, the sensitivity filtering scheme [Sigmund (2001)] has been widely used to achieve a checkerboard-free and meshindependency design in the topology optimization of continua, which modified the design sensitivities during iterations as follows:

$$\frac{\partial c}{\partial x_e} = \frac{1}{x_e \sum_{f=1}^N H_f} \sum_{f=1}^N H_f x_f \frac{\partial c}{\partial x_f}$$
(4)

where the subscript f satisfies $\{f \in N | dist(e, f) \le r_{min}\}, e=1, ..., N. dist(e, f)$ is defined as the distance between the center of element e and center of element f, r_{min} is the filter radius. \bigwedge^{\wedge}_{f} is written as

$$\stackrel{\wedge}{H_f} = r_{\min} - dist(e, f) \tag{5}$$

This method makes the design sensitivity of a specific element depend on a weighted average around the element's neighbors that located within the scope of the radius dist(e, f). Because of the weighted average operation, a specific element's density will be repeatedly evaluated many times. The direct side-effect is it will lead to gray-scale elements, although is it can avoid the checkerboards efficiently. In particular, with the increasing of the radius dist(e, f), the gray-scale becomes more serious.

3 Modified optimality criterion methods

3.1 Optimality criterion method to update element densities

One of the difficulties in topology optimization of continua is a large-scale number of design variables to be updated iteratively. An efficient optimization algorithm is important for a given problem. Many methods have been developed as the optimizers for topological optimization problems, including the Optimality Criterion (OC) methods [Rozvany, Bendsøe and Kirsch (1995)]. The OC method realizes the optimization through establishing the optimality criterion and the iteration formula, with advantages including the fast convergence, as well as the complexity level has no association with the structural re-analysis and the number of variables. In this paper, the scheme of updating element densities is based on the OC method, which can be written as

$$x_{new} = \begin{cases} \max(x_{\min}, x_e - m) \\ \text{if } x_e B_e^{\eta} \le \max(x_{\min}, x_e - m) \\ x_e B_e^{\eta} \\ \text{if } \max(x_{\min}, x_e - m) \le x_e B_e^{\eta} \le \min(1, x_e + m) \\ \min(1, x_e + m) \\ \text{if } \min(1, x_e + m) \le x_e B_e^{\eta} \end{cases}$$
(6)

where *m* is a positive small constant to be used as a move-limit. η is a numerical damping coefficient (typically the value is 1/2), and B_e is defined as follows:

$$B_e = \frac{-\frac{\partial c}{\partial x_e}}{\lambda \frac{\partial V}{\partial x_e}} \tag{7}$$

where λ is a Lagrangian multiplier that can be found by a bi-sectioning algorithm. The sensitivity of the objective function is found as

$$\frac{\partial c}{\partial x_e} = -p(x_e)^{p-1} u_e^T k_0 u_e \tag{8}$$

In order to ensure existence of solutions to the topology optimization, Eq. (6) will be in association with the OC method to update elemental densities, in order to obtain a meaningful solution without experiencing the typical numerical instabilities.

3.2 Modified optimality criterion method

From Section 2, it can be seen that it is improper to delete too many elements of relative densities between 0.5 and 1.0. In order to get a better result, it is important to find a penalty function that makes the elements whose relative densities are lower than 0.5 close to 0, and the elements with relative densities higher than 0.5 close to 1.0. This will reduce the gray-scale elements somewhat.

Based on this concept, this paper proposes two different heuristic formulas for construct modified OC methods to suppress gray-scale elements. The main idea is to weaken the effect of low-relative-density elements and enhance the contribution of high-relative-density elements. In each optimization step, one of the heuristic methods will be included after updating the elements' densities by Eq.(6). The result is to make design variables close 0 or 1. These methods can not only suppress the gray-scale elements, but also accelerate the convergence. The mathematical formulas of these two methods can be written as

$$x'_{new} = \frac{e^{(-\frac{\omega}{2} + ax_{new})}}{1 + e^{(-\frac{a}{2} + ax_{new})}}$$
(9)

$$x'_{new} = \frac{2.55 \arctan[b(2x_{new} - 1)]}{4(1 + e^{-\frac{x_{new}}{b}})} + \frac{1}{2}$$
(10)

where x_{new} and x'_{new} are the element densities after using the OC method, given in Eq. (6) and Eq. (9) or Eq. (10), respectively. *a* or *b* is the parameter that controls the polarization level (steepness parameter). Fig. 2 is the graphs of Eq. (9) and Eq. (10) with different steepness parameters *a* and *b*.



Figure 2: Graphs of the two heuristic formulas

As Fig. 2 shows, these two methods can make the intermediate densities materials approach to 0 or 1. With the increasing of the steepness parameters, the curves are approximately close to a smoothed Heaviside step function. The smoothed Heaviside function can get better results when they are included to update the element densities. In this way, the low-relative-density elements are weakened and the corresponding stiffness matrixes are weakened, so the inference to the global stiffness matrix can be ignored because of the relative density contribution is very lower. For the high-relative-density elements, the effect is opposite, which means that their corresponding stiffness matrixes are enhanced.

3.3 Convergence criterion

The choice of convergence criterion is also important to the topology optimization. Based on the Modified OC methods, convergence strategy of this paper is introduced as follows:

$$\left|\frac{C^{(k+1)} - C^{(k)}}{C^{(k)}}\right| \le \varepsilon \tag{11}$$

where $C^{(K+1)}$ and C^K are the compliance of the (K+1)th and *K*th iteration, respectively. This convergence strategy contains two stages:

(1) At early stage of the iteration, in order to prevent the subsequent optimization being influenced by low-relative-density elements, a lower-relative steepness parameter (for example, a=8 or b=3) is applied until Eq. (11) is satisfied, where the value of ε is 0.3%.

(2) After the first stage, most elements' densities approximate to either 1 or the lowest density value, to get a faster convergence speed, adopting a higher-relative steepness parameter (for example, a=18 or b=8), until the convergence condition given in Eq. (11) is satisfied, where ε is 0.1%.

4 Flowchart of modified optimality criterion method

The flowchart of the modified optimality criterion method is displayed in Fig. 3. As indicated in Fig. 3, the whole process contains five steps, and each step will be explained as follows:

(1) Set the initial value. Define the design domain, material's property and load parameters, and then discretize the design domain with finite elements.

(2) Structural analysis. Finite Element Method is applied to structural numerical analysis. Set boundary conditions, define loads, construct elemental stiffness matrix, assemble the global stiffness matrix, and then solve the state equation.

(3) Optimization. In this step, the optimization is performed using one of the Modified OC methods. During the optimization, the variables are updated, and the process is being processed until the corresponding convergence criterion is satisfied.

(4) Convergence. If the design meets the convergence criterion, the design is convergent and the optimization will stop. Otherwise, it will return to the second step to continue the optimization.

5 Numerical examples

Numerical examples are presented in this section to demonstrate the availability and efficiency of the Modified OC method in topology optimization. The following will present two typical numerical examples. One is the cantilever and the other is the



Figure 3: Flowchart of modified optimality criterion method

half MBB. In each example, three methods will be used to solve the given problem: the conventional OC and the two Modified OC methods. These examples are based on the 99 line topology optimization MATLAB code by [Sigmund (2001)].

5.1 Numerical example 1: The optimization of the cantilever

As indicated in Fig. 4, the design domain of the problem is a $0.4m \times 0.25m$ rectangle with a thickness of 0.01m, discretized with 80×50 quadrilateral finite elements of low order. The load *P* is 1000 N, located at the middle point of the right side of the structure. The left side of the structure is fixed. All necessary parameters for the optimization are listed in Table 1.

Table 2 shows the optimal topologies and corresponding steps with different meth-



Figure 4: Design domain with working conditions of the cantilever

Parameter	Value	Meaning
Ε	2.10×10^{11}	Young's module
μ	0.3	Poisson's ratio
р	3.0	penalty factor
r	2.5	filter radius
f	0.5	volume fraction
ρ_0	[1,1,,1]	Initial values

Table 1: Parameters for topology optimization

ods. From Table 2, it can be seen that the Modified OC methods can produce better optimal topologies: lower compliance and lesser iterations. As mentioned in Section 3.2, in the process of updating elemental densities, Eq. (9) and Eq. (10) can reasonably make the design variables close to 0 or 1, instead of deleting too many elements of relative densities between 0.5 and 1.0. Furthermore, since the strategy of different convergence criteria are employed in this paper at different stages, the Modified OC methods can automatically choose different predefined steepness parameters. These might be the reason why the compliances are lower and the iteration numbers are lesser than the conventional OC method.

In addition, the major merit is the boundary of final topological designs is distinct because of the gray-scale elements are greatly suppressed, when the Eq. (9) or Eq. (10) are combined with the OC method to solve the problem. As shown by Fig. 6, the conventional OC method lead to 508 gray-scale elements with intermediate material densities (relative density between 0.2 and 0.8) in total, while the modified two OC methods are 0 in this given problem, respectively. Table 3 is the snap-shots of the topological designs obtained at different design stages. It shows that both Modified OC methods can generate good topology designs with faster speed

compared to the conventional OC method.

This example exhibits that the two Modified OC methods can be used to solve topology optimization problems subject to single constraints with higher numerical accuracy and fast convergence.

 Table 2: Comparison between OC method and two Modified OC methods

Method	The OC method	The first Modified OC method	The second Modified OC method
Optimal topologies	$\mathbf{\Sigma}$	$\mathbf{\Sigma}$	$\mathbf{\Sigma}$
Volume fraction	0.5	0.5	0.5
Steepness parameters		a1=7.0 a2=20.0	b1=3.5 b2=10.0
Compliance ($\times 10^3$ /J)	192.266	177.837	190.809
Iteration steps	20	15	17

Table 3: Snapshots of the topology obtained at different iteration steps.

Method	The OC method	The first Modified OC method	The second Modified OC method
t=5		X	\otimes
t=10	$\mathbf{\Sigma}$	$\mathbf{\Sigma}$	\gg
t=15	\mathbf{X}	$\mathbf{\Sigma}$	\mathbf{X}

5.2 Numerical example 2: The optimization of the half MBB-beam

The second example is shown in Fig. 6, which is further used to demonstrate the effectiveness of the proposed OC methods. The design domain is a $0.45m \times 0.15m$ rectangle area with a thickness of 0.01m, discretized by 90×30 quadrilateral finite



Figure 5: The histogram of elements number in different relative density interval



Figure 6: Design domain of the half MBB-beam

elements for structural analysis. The load P is 1000 N, located at the middle point of the upper side. In the numerical implementation, only half "MBB-beam" is used to take advantage of structural symmetry. In the symmetric design domain, the load is applied vertically in the upper left corner and the lower right corner is simply supported, and the left edge is regarded as the symmetric boundary condition. All parameters are listed in Table 4.

Parameter	Value	Meaning
E	2.10×10^{11}	Young's module
μ	0.3	Poisson's ratio
p	3.0	penalty factor
r	3.75	filter radius
f	0.5	volume fraction
$ ho_0$	[1,1,,1]	Initial values

Table 4: Parameters for the problem in Fig. 6

Table 5 displays the results using different OC methods in the optimization. The optimal topologies and the corresponding iterations indicate that the proposed methodology can lead to topological designs with distinct boundaries and the optimization converges relatively fast. So the number of gray-scale elements (relative densities between 0.2 and 0.8) are less than that of the conventional OC method. That is, the conventional OC method produced 629 gray-scale elements, while the proposed first and the second Modified OC methods are 2 and 27, respectively, as denoted by Fig. 7. Table 6 shows that the Modified OC methods can converge relatively fast.

Method	The OC method	The first Modified OC method	The second Modified OC method
Optimal topologies	\sim	\sim	$\mathbf{\Sigma}$
Volume Steepness	0.5	0.5 a1=9.0 a2=22.0	0.5 b1=4.9 b2=15.0
Compliance $(\times 10^3/J)$	1059.822	923.831	1052.229
Iteration steps	27	20	25

Table 5: Comparison between OC and two Modified OC methods



Figure 7: The histogram of elements number in different relative density interval



Table 6: Topologies obtained at different iteration steps (t)

From the above discussions, it can be seen that the Modified OC methods can efficiently suppress the gray-scale elements in the topology optimization of continuum structures, which is greatly beneficial to designers in reasonably extracting black-white boundaries without over or under estimations. Both methods can lead to better topological designs with lower compliances (or higher stiffness), and the numerical convergence is relatively fast than the conventional OC method. Our ongoing research is to achieve topological designs with distinct but more smoothed boundaries.

6 Discussion and conclusions

The unique characteristic of the proposed methodology is it can create topological designs with distinct boundaries with materials either close to 0 (void) or 1 (solid), besides its abilities to avoid typical numerical instabilities including checkerboards and mesh-dependency. From the numerical results, it can be found that the two Modified OC methods can efficiently suppress gray-scale elements in the final designs. The optimal designs can be obtained only through relatively a small number of iterations in terms of the explicit approximation and sensitivity analysis involved in OC methods.

It should be pointed out that each Modified OC method employs a steepness parameter to ensure the convergence of the iteration, and the parameter has a direct effect on the convergence and accuracy of the algorithm. More or less, it is a matter of numerical experience to properly choose a or b to make the convergence quicker and more accurate. The methods proposed in this study can be extended to handle more complex topology optimization problems of continua.

Acknowledgement: This research was partially supported by the National Natural-Science-Foundation-of-China (51105229), Natural-Science-Foundation-of-Hubei-Province, China (2010CDB1085), and Open Fund of Hubei Key Laboratory of Hydroelectric Machinery Design and Maintenance (2010KJX04).

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