Application of Order-Preserving Functions to the Modeling of Computational Mechanics Problems with Uncertainty^{*}

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Abstract

In many engineering problems the shape of the structure is not exactly known. In that situation it is possible to consider a family of shapes which belong to the interval set $\Omega \in [\underline{\Omega}, \overline{\Omega}]$. In order to find upper and lower bound of the solution, which depend on uncertain (interval) shape, it is possible to use properties of topological derivative or differentials which are positive definite (in many cases positive definite differentials are simply positive). Numerical examples are related to the heat transfer, imprecise probability, and integration on manifolds.

Keywords: Interval parameters, interval sets, imprecise probability, topological derivative, uncertainty.

AMS subject classifications: 65G30, 65G40, 68T37, 35Q80, 54H99

1 Set uncertainty in computational mechanics

Many parameters of engineering structures are not known exactly [15]. Mathematical models of mechanical systems are usually built using systems of equations (partial differential equations, algebraic equations, integral equations etc.) with different parameters. From a mathematical point of view it is necessary to know several numbers, functions, and sets. If this information is uncertain, it is necessary to apply appropriate methods for modeling of uncertainty.

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Parameter type	Non-probabilistic methods	Probabilistic methods
numbers	interval numbers	random numbers
functions	interval functions	random fields
sets	interval sets	random sets, clouds

Table 1: Methods of modeling of uncertainty

Let us consider $T = T(x, \Omega, k, q(x))$, which is a solution of the heat transfer equation:

$$k\left(\frac{\partial^2 T}{\partial x_1^2} + \frac{\partial^2 T}{\partial x_2^2} + \frac{\partial^2 T}{\partial x_3^2}\right) + q = 0, \quad x \in \Omega,$$

$$T(x) = T^*(x), \quad x \in \partial\Omega.$$
 (1)

where T = T(x) is temperature in the region $\Omega \subset \mathbb{R}^3$. $T = T^*(x)$ is known temperature on the boundary $\partial\Omega$, k is heat conductivity, and q is the heat source. In this example k is a number and can be described by a real number, interval number [2], random number, and cloud [1]. Heat source q can be represented by a function, interval function [4], or random field [8]. The set Ω in the presence of uncertainty can be described by using interval set $\hat{\Omega} = [\Omega, \overline{\Omega}]$ [4]. This interval set is defined with the order relation \leq .

$$\hat{\Omega} = \{\Omega : \underline{\Omega} \leqslant \Omega \leqslant \overline{\Omega}\}.$$
(2)

$$A \leqslant B \Leftrightarrow A \subseteq B. \tag{3}$$

In this paper only the case of set uncertainty will be presented. In that case upper and lower bound of the solution can be defined in the following way:

$$\begin{cases} \frac{T(x) = \min\{T(x, \Omega) : \Omega \in [\underline{\Omega}, \overline{\Omega}]\},\\ \overline{T}(x) = \max\{T(x, \Omega) : \Omega \in [\underline{\Omega}, \overline{\Omega}]\} \end{cases}$$
(4)

$$T(x,\Omega) \in [\underline{T}(x),\overline{T}(x)]$$
 (5)

Interval parameters and interval functions are discussed in the papers [4, 9]. A longer list of references and web applications, which are able to solve computational mechanics problems with the interval parameters, can be found on the web page http://andrzej.pownuk.com.

2 Classical definition of topological derivative

Let us consider an open, bounded domain, $\Omega \subset \mathbb{R}^n$ (n=1,2,3) with a smooth boundary $\partial\Omega$. If the domain is perturbed by introducing a small hole B_{ε} of radius ε at the arbitrary point $x \in \Omega$, we have new domain $\Omega_{\varepsilon} = \Omega - \overline{B}_{\varepsilon}$, whose boundary is denoted by $\partial\Omega_{\varepsilon} = \partial\Omega \cup \partial B_{\varepsilon}$. Topological derivative of certain cost function $\psi = \psi(\Omega)$ can be defined as the following limit [11]

$$D_T(x) = \lim_{\varepsilon \to 0^+} \frac{\psi(\Omega_\varepsilon) - \psi(\Omega)}{f(\varepsilon)}$$
(6)

where $f(\varepsilon)$ is a given function, which is positive $(f(\varepsilon) > 0)$ and

$$\lim_{\varepsilon \to 0^+} f(\varepsilon) = 0. \tag{7}$$

If $f(\varepsilon)=|B_\varepsilon|$ (where $|B_\varepsilon|=\int\limits_{B_\varepsilon}d\Omega$) then we can use the following notation

$$D_T(x) = \frac{d\psi}{d\Omega(x)} \tag{8}$$

3 Parametric method for calculating topological derivative

It is also possible to define topological derivative for completely arbitrary perturbations. In this case, Ω_{ε} is the arbitrary set (i.e. not necessarily $\Omega_{\varepsilon} = \Omega - \bar{B}_{\varepsilon}$). However $\Omega_{\theta} \to \Omega$, when $\theta \to 0$.

$$D_T(x) = \lim_{\theta \to 0} \frac{\psi(\Omega_\theta) - \psi(\Omega)}{f(\theta)} =$$
(9)

$$= \lim_{\theta \to 0} \frac{\frac{\psi(\Omega_{\theta}) - \psi(\Omega)}{\theta}}{\frac{f(\varepsilon) - f(0)}{\theta}} = \left(\frac{\frac{d\psi}{d\theta}}{\frac{df}{d\theta}}\right)_{\theta = 0} = D_T^{(\theta)}(x)$$
(10)

In some cases, the formula (10) gives the same results for different parameterizations (ε) .

Let us consider a triangle *ABC*, where *A*=(0,0), *B*=(1,0), *C*=(1+ ε ,1). and a function $\psi_1(\varepsilon) = \psi_1(\Omega_{\varepsilon}) = |\Omega_{\varepsilon}|^2$, where $|\Omega_{\varepsilon}| = (1 + \varepsilon)/2$ is the area of the triangle, $f(\varepsilon) = |\Omega_{\varepsilon}| - 0.5$.

$$D_T^{\varepsilon} = \left(\frac{\frac{d\psi_1}{d\varepsilon}}{\frac{df}{d\varepsilon}}\right)_{\varepsilon=0} = \left(\frac{\frac{1+\varepsilon}{2}}{\frac{1}{2}}\right)_{\varepsilon=0} = 1.0$$
(11)

In this case, topological derivative can be calculated for all parameterizations

$$\lim_{\varepsilon \to 0^+} \frac{\psi_1(\Omega_\varepsilon) - \psi_1(\Omega)}{f(\varepsilon)} = \lim_{\varepsilon \to 0^+} \frac{|\Omega_\varepsilon|^2 - 0.5^2}{|\Omega_\varepsilon| - 0.5} =$$
(12)

$$\lim_{\varepsilon \to 0^+} |\Omega_{\varepsilon}| + 0.5 = |\Omega_0| + 0.5 = 1$$
(13)

Let us consider the function $\psi_2(\Omega_{\varepsilon}) = y_C = \varepsilon$, for the parameterization which was given above

$$D_T^{\varepsilon} = \left(\frac{\frac{d\psi_2}{d\varepsilon}}{\frac{df}{d\varepsilon}}\right)_{\varepsilon=0} = \left(\frac{1}{\frac{1}{2}}\right)_{\varepsilon=0} = 2$$
(14)

Let us consider different parameterization of the shape of the triangle $C=(1+\gamma,1)$. In this case, $\psi_2(\Omega_{\gamma}) = y_C = 1$

$$D_T^{\gamma} = \left(\frac{\frac{d\psi_2}{d\gamma}}{\frac{df}{d\gamma}}\right)_{\gamma=0} = \left(\frac{0}{\frac{1}{2}}\right)_{\varepsilon=0} = 0 \tag{15}$$

Then $2 = D_T^{\varepsilon} \neq D_T^{\gamma} = 0$ i.e. the result depends on the parameterization. In the literature, usually the concept of parameter independent topological derivative is used [5, 6, 10].

Example If $f(\Omega) = \int_{\Omega} f(x) d\Omega(x)$ then $df(\Omega, \Delta \Omega_x) = f(x) |\Delta \Omega_x|,$ (16)

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$$\frac{df}{d\Omega(x)} = f(x) \tag{17}$$

Example

In general if the function $f(\Omega) = F\left(\int_{\Omega} L(x)d\Omega\right)$ where F is some function, then

$$df(\Omega, \Delta\Omega_x) = F'\left(\int_{\Omega} L(x)d\Omega\right) L(x)|\Delta\Omega_x|,$$
(18)

$$\frac{df}{d\Omega(x)} = F'\left(\int_{\Omega} L(x)d\Omega\right)L(x).$$
(19)

Let $f(\Omega)$ is center of gravity of the set Ω i.e.

$$f(\Omega) = \frac{\int x d\Omega}{\int \Omega d\Omega},$$
(20)

then topological derivative is equal to

$$\frac{df}{d\Omega(x)} = \frac{x \int_{\Omega} d\Omega - \int_{\Omega} x d\Omega}{\left(\int_{\Omega} d\Omega\right)^2} = \frac{x |\Omega| - \int_{\Omega} x d\Omega}{|\Omega|^2}.$$
(21)

4 Example - center of gravity of the region with uncertain shape

Let us consider a region with uncertain shape which is shown in the Fig. 1. It is possible to calculate upper and lower bounds of center of gravity of the region with uncertain shape by using topological derivative (21). The method was implemented in Java and can be applied to the region with arbitrarily uncertainty and uncertain shape (compare Fig. 1).



Figure 1: Program which calculates upper and lower bounds of the center of gravity (written in Java)

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5 General approach to monotonicity based on the sign of differential

Function is monotone if

$$x \leqslant y \Rightarrow f(x) \leqslant f(y) \tag{22}$$

or strictly monotone if

$$x < y \Rightarrow f(x) < f(y) \tag{23}$$

where \leq is a partial order relation and < is a strict partial order [7, 12].

Between two A and B it is possible to define the following partial order relation +.

$$A \leqslant B \Leftrightarrow A \subseteq B \tag{24}$$

and addition +.

$$A + B \Leftrightarrow A \cup B \tag{25}$$

It is clear that $\Omega + \Delta \Omega_x \ge \Omega$.

Differential is possitive definite if exists $\varepsilon > 0$ such that

$$df(\Omega, \Delta\Omega_x) \ge c |\Delta\Omega_x| \quad for \quad all \ \rho(\Delta\Omega_x) < \varepsilon \tag{26}$$

Differential is possitive if exists $\varepsilon > 0$ such that

$$df(\Omega, \Delta\Omega_x) \ge 0 \quad for \quad all \ \rho(\Delta\Omega_x) < \varepsilon \tag{27}$$

Theorem If $\varepsilon > 0$ exists such that $df(\Omega, \Delta\Omega_x) \ge c |\Delta\Omega_x|$ for all $\rho(\Delta\Omega_x) < \varepsilon$, then $\delta > 0$ exists such that $f(\Omega + \Delta\Omega_x) \ge f(\Omega)$ for all $\rho(\Delta\Omega_x) < \delta$.

 $\mathbf{Proof} \ \mathbf{Because}$

$$\lim_{\rho(\Delta\Omega_x)\to 0} \frac{|R(\Omega, \Delta\Omega_x)|}{|\Delta\Omega_x|} = 0$$
(28)

then for each $\varepsilon > 0$ exists $\delta > 0$ such that

$$|R(\Omega, \Delta\Omega_x)| \leq |\Delta\Omega_x|\varepsilon \quad for \quad \rho(\Delta\Omega_x) < \delta; \tag{29}$$

in other words

$$R(\Omega, \Delta\Omega_x) \ge -|\Delta\Omega_x|\varepsilon \quad for \quad \rho(\Delta\Omega_x) < \delta \tag{30}$$

Now it is possible to estimate the sign of the finite difference $\Delta f(\Omega, \Delta \Omega_x)$

$$\Delta f(\Omega, \Delta \Omega_x) = f(\Omega + \Delta \Omega_x) - f(\Omega) = df(\Omega, \Delta \Omega_x) + R(\Omega, \Delta \Omega_x)$$
(31)

$$df(\Omega, \Delta\Omega_x) + R(\Omega, \Delta\Omega_x) \ge c|\Delta\Omega_x| + R(\Omega, \Delta\Omega_x) \ge c|\Delta\Omega_x| - \varepsilon|\Delta\Omega_x|$$
(32)

$$f(\Omega + \Delta\Omega_x) - f(\Omega) \ge (c - \varepsilon) |\Delta\Omega_x|$$
(33)

Let us assume that $\varepsilon = \frac{c}{2}$ then

$$f(\Omega + \Delta\Omega_x) - f(\Omega) \ge \left(c - \frac{c}{2}\right) |\Delta\Omega_x| = \frac{c}{2} |\Delta\Omega_x| \ge 0.$$
(34)

Hence

$$f(\Omega + \Delta \Omega_x) \ge f(\Omega). \tag{35}$$

Important remark In many cases positive differential $df(\Omega, \Delta\Omega_x)$ is also positive definite and in that case it is enough to study the sign of the differential instead of positive definiteness.

This theorem can be applied to the optimization of the function, which depends on the sets. For sufficiently small increments $\Delta \Omega_x$ the value of differential can be approximated by the difference.

$$df(\Omega, \Delta\Omega_x) \approx f(\Omega + \Delta\Omega_x) - f(\Omega) = \Delta f(\Omega, \Delta\Omega_x)$$
(36)

It is obvious that if $\Delta f(\Omega, \Delta \Omega_x) \ge 0$ for all $\rho(\Delta \Omega_x) < \varepsilon$, then the function $f(\Omega + \Delta \Omega_x) \ge f(\Omega)$ for all increments $\rho(\Delta \Omega_x) < \varepsilon$ (i.e. $\delta = \varepsilon$).

6 Extreme values of the integrals on manifolds

Let us consider manifold M, differential form ω , and some set $\Omega \subset M$.

$$f(\Omega) = \int_{\Omega} \omega. \tag{37}$$

Differential form the function $f(\Omega)$ is equal to

$$df(\Omega, \Delta\Omega_x) = \omega(x, \Delta\Omega_x). \tag{38}$$

Example - line integral from scalar field

Let $f(\Omega) = \int_{\Omega} L(x) dt$ then differential is equal to $df(x, \Delta\Omega_x) = L(x) |\Delta\Omega_x|$. It is clear that if L(x) > 0 then df > 0 and $\underline{f} = f(\Omega^{min}), \overline{f} = f(\Omega^{max})$ where Ω^{min} is the smallest set, and Ω^{max} is the biggest set (i.e. $\Omega^{min} = \underline{\Omega}, \Omega^{max} = \overline{\Omega}$ where $\Omega \in [\underline{\Omega}, \overline{\Omega}]$).

Example - line integral from vector field

Let $f(\Omega) = \int_{\Omega} P(x,y)dx + Q(x,y)dy$ then differential is equal to $df(x,y,\Delta\Omega_{x,y}) = P(x,y)|\Delta x| + Q(x,y)|\Delta y|$. If $df(x,y,\Delta\Omega_{x,y}) > 0$ for all considered points x, y then $\underline{f} = f(\Omega^{min}), f^u = f(\Omega^{max})$ where Ω^{min} is the smallest set, and Ω^{max} is the biggest set (i.e. $\Omega^{min} = \underline{\Omega}, \Omega^{max} = \overline{\Omega}$ where $\Omega \in [\underline{\Omega}, \overline{\Omega}]$).

Example - surface integral

Let us consider surface integral $f(\Omega) = \int_{\Omega} L(x, y, z) dS$ where $L(x, y, z) \ge 0$ for all $(x, y, z) \in \Omega$. $df(x, y, z, \Delta\Omega_{x,y,z}) = L(x, y, z) |\Delta\Omega_{x,y,z}| > 0$ for all considered points x, y then $\underline{f} = f(\Omega^{min}), \overline{f} = f(\Omega^{max})$ where Ω^{min} is the smallest set, and Ω^{max} is the biggest set (i.e. $\Omega^{min} = \overline{\Omega}, \Omega^{max} = \underline{\Omega}$ where $\Omega \in [\underline{\Omega}, \overline{\Omega}]$).

7 Upper and lower bound of the solution of PDE with uncertain set-valued parameters

Let us consider boundary value problem

$$\begin{cases} F(x,T(x)) = 0, & x \in \Omega\\ B(x,T(x)) = 0, & x \in \partial \Omega \end{cases}$$
(39)

Solution of that BVP depends on the set Ω i.e. $T = T(x, \Omega)$. In many applications the shape of the set Ω is uncertain. In order to describe that uncertainty it is possible to use the interval sets i.e. $\Omega \in [\underline{\Omega}, \overline{\Omega}]$. Upper and lower bounds of the solution are defined in the equation (4). In order to find upper and lower bound of the solution it is possible to use the concepts of topological derivatives and continuous gradient methods.

Calculation of the upper bound $\overline{T}(x_0)$

1) Set initial shape $\Omega = \Omega_0$ and $x = x_0$.

2) Discretize the uncertain region $\tilde{\Omega} = \underline{\Omega} \cap \overline{\Omega}$ initial shape and replace it by a set of discrete values $\tilde{\Omega} = \Delta \Omega_{x_1} \cup ... \cup \Delta \Omega_{x_n}$.

3) Find the elements $\Delta\Omega_{x_i}$ which are next to the boundary $\partial\Omega$. Let's denote all the boundary elements which belong the uncertain region by $\partial\tilde{\Omega} = \Delta\Omega_{x_{i1}} \cup ... \cup \Delta\Omega_{x_{im}}$.

4) For all elements which belong to the boundary $\partial \tilde{\Omega}$ calculate the differential $dT(x, \Omega, \Delta \Omega_{x_i}) \approx T(x, \Omega) - T(x, \Omega - \Delta \Omega_{x_i})$.

5) Remove all elements from the list $\partial \tilde{\Omega}$ for which dT < 0. Let us denote the new list as $\partial \tilde{\Omega}^{max}$.

6) Create new shape Ω_{new} which has the boundary $\partial \tilde{\Omega}^{max}$.

7) If all sets in the list $\partial \tilde{\Omega}$ are smaller than given ε , then stop the calculations.

8) If new shape Ω_{new} is the same like as the old shape Ω then $T^u(x) = T(x, \Omega)$ and stop the calculation other vice $\Omega = \Omega_{new}$ and go to step 3.

Similar methods can be applied for calculation of lower bound $\underline{T}(x)$ of the solution. That procedure has to be repeated for each point x. In general this is a very high dimensional and time consuming problem. Fortunately it is possible to apply the concept of sign vectors [3, 4], which reduce the time of calculations significantly.

8 Numerical example: heat transfer with uncertain geometry

Let us consider 2D stationary heat transfer problem with Dirichlet boundary conditions

$$\frac{\partial}{\partial x} \left(k_x \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(k_y \frac{\partial T}{\partial y} \right) + q = 0, \quad (x, y) \in \Omega$$

$$T(x, y) = T^*(x, y), \quad (x, y) \in \partial\Omega$$
(40)

In numerical example (40) Ω is a rectangular region with the dimension 2×2 . Uncertainty is shown in the Fig. 2 and represent rectangular region with dimension 0.5×0.5 . Temperature is the same on the whole boundary and it is equal to 10. Heat source is in the middle of the region and it is equal to 10. Boundary value problem (40) was solved by using FDM method. The method was implemented in C++ language. This program is using special scripting language. Presented examples can be described using a set of commands.

CreateRegion 0,0 2,2 9,9

 SetBoudaryCondition
 0
 0
 2
 10
 10

 SetBoudaryCondition
 0
 2
 2
 2
 10
 10

 SetBoudaryCondition
 2
 2
 2
 0
 10
 10

 SetBoudaryCondition
 2
 2
 0
 10
 10

 SetBoudaryCondition
 2
 0
 0
 10
 10



Figure 2: Uncertainty

SetKx SetKy SetQ	1.0 1.0 1 1 10.0						
Solve							
SaveInde	ex	index.txt					
SaveRegi	ionValues	solution0.txt					
SetUncer	rtainty	0 0 0.5 0.5					
SaveUnce	ertainty	uncertainty.txt					
Calculat	ceSensitivity						
SaveMins	Solution	MinSolution.txt					
SaveMins	SolutionIndex	MinIndexSolution.txt					
SaveMaxS	Solution	MaxSolution.txt					
SaveMaxS	SolutionIndex	MaxIndexSolution.txt					

Interval solution is shown on the Fig. 3, maximal solution on the Fig. 4.

Internal representation of perturbed region is given on the Fig. 5.

Numerical experiments showed that the solution is very monotone with respect to changes of the shape. Upper and lower bounds are given by two shapes for all points in the region $\Omega - \tilde{\Omega}$. In order to find the solution it is necessary to solve only two problems:

$$\underline{T}(x) = T(x, \Omega^{min}), \quad \overline{T}(x) = T(x, \Omega^{max}).$$
(41)



Figure 3: Interval solution



Figure 4: Upper bound on the solution

1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
1	0	0	0	0	0	0	0	0	0	0	0	0	0	1
1	0	0	0	0	0	0	0	0	0	0	0	0	0	1
1	1	0	0	0	0	0	0	0	0	0	0	0	0	1
1	0	0	0	0	0	0	0	0	0	0	0	0	0	1
1	0	0	0	0	0	0	0	0	0	0	0	0	0	1
1	0	0	0	0	0	0	0	0	0	0	0	0	0	1
1	0	0	0	0	0	0	0	0	0	0	0	0	0	1
1	0	0	0	0	0	0	0	0	0	0	0	0	0	1
1	0	0	0	0	0	0	0	0	0	0	0	0	0	1
1	0	0	0	0	0	0	0	0	0	0	0	0	0	1
1	0	0	0	0	0	0	0	0	0	0	0	0	0	1
1	0	0	0	0	0	0	0	0	0	0	0	0	0	1
1	0	0	0	0	0	0	0	0	0	0	0	0	0	1
1	1	1	1	1	1	1	1	1	1	1	1	1	1	1

Figure 5: Internal representation of perturbed region

9 Reliability of structures with uncertain shape

Reliability of engineering structures can be calculated as

$$P_f = P\{g(x) \leqslant 0\} \tag{42}$$

If the structure has interval parameters \hat{p}_i then probability belongs to the interval [14]

$$\hat{P}_f = [\underline{P}_f, \overline{P}_f] = \{ P_f(p_1, ..., p_m) : p_1 \in \hat{p}_1, ..., p_m \in \hat{p}_m \}$$
(43)

of failure with interval parameters is presented in the paper. Similarly if the shape of the structure Ω is uncertain (i.e. $\Omega \in [\underline{\Omega}, \overline{\Omega}]$) then probability of failure also belongs to the interval $P_f \in [\underline{P}_f, \overline{P}_f] = \{P_f(\Omega) : \Omega \in [\underline{\Omega}, \overline{\Omega}]\}$. Extreme values of the probability of failure can be calculated by using topological derivative or differential and sensitivity analysis or continuous version of gradient method [3, 4].

$$dP_f(\Omega, \Delta\Omega_x) \approx P_f(\Omega + \Delta\Omega_x) - P_f(\Omega) = \Delta P_f(\Omega, \Delta\Omega_x)$$
(44)

Example

Let us consider some abstract problem in which the probability of failure can be calculated by using the following criteria:

$$P_f(\Omega) = \left(\int_{\Omega} L(x)d\Omega\right)^2 \tag{45}$$

where $L(x) \ge 0$ $(0 \le P_f(\Omega) \le 1$ for all $\Omega \in [\underline{\Omega}, \overline{\Omega}]$ and $\Omega \in [\underline{\Omega}, \overline{\Omega}] = \hat{\Omega}$. Differential can be calculated in the following way:

$$dP_f(\Omega, \Delta\Omega_x) = 2\left(\int_{\Omega} L(x)d\Omega\right) \cdot |\Delta\Omega_x| \ge 0$$
(46)

Because the differential is always positive then $\Omega^{min} = \underline{\Omega}, \Omega^{max} = \overline{\Omega}$ and

$$\underline{P}_f = P_f(\Omega^{min}) = P_f(\underline{\Omega}), \quad \underline{P}_f = P_f(\Omega^{max}) = P_f(\overline{\Omega})$$
(47)

Then probability of failure belongs to the following interval $P_f \in [\underline{P}_f, \overline{P}_f]$.

10 Conclusions

Using the sign of differential and topological derivative it is possible to efficiently solve many problems of computational mechanics with uncertain shapes. Techniques which are based on sign vectors significantly reduce the time of calculations. According to numerical results the relation between the solution of heat transfer problem and the shape is monotone. In the case of the center of gravity the relation between the shape of the region and the center of gravity is more complicated and it is necessary to apply continuous version of gradient method. More complicated examples can be found in the paper [13].

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