NUMERICAL SOLUTION OF A SHAPE OPTIMIZATION PROBLEM

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ABSTRACT

This paper is concerned with the identification of the geometric structure of the boundary for a two-dimensional (stationary) elliptic equation. The domain identification problem is considered as a variational problem to minimize a defect functional, which utilizes some additional data on certain (known) parts of the boundary. The Gradient Projection Method is introduced for this problem and numerical results for two model examples are discussed.

1. INTRODUCTION

Shape optimatization problems are important in determining the domain of corroding materials and the location of cracks in electrical conductors, for the optimal design of aerospace structures and airfoil wings, optimization of electromagnets, thermal tomography and for many other applications (e. g. [1]). In this paper, domain identification for elliptic equations in two spatial variables is studied where parts of the boundary have to be determined by sufficient conditions on other parts. Such problems are highly nonlinear and they are well known to be ill-posed. The latter means that small perturbations in the data can cause large errors in the solutions. For numerical methods, discretization and truncation errors may also lead to useless results.

In the literature, existence and uniqueness of such problems are studied (s. [2]). Moreover, stability results in form of logarithmic stability estimates are available (cf. [3], [4]). Several computational results can be found in the literature using, e.g., Tikhonov regularisation in connection with the L-curve method to determine the regularisation parameter (e. g. [5]).

In this paper we propose a variational method: We consider the unknown parameter vector as a control to minimize a defect functional. The Gradient Projection Method is used to solve the problem iteratively, where the gradient of the minimizing functional is also determined numerically. In our iterative procedure the iteration index plays the role of a regularization parameter [6]. Suitable stopping criteria, as the Morozov and Nemirowskii stop-

ping rule [7], [8] can be applied to determine the optimal stopping index.

Our approach differs from the 'method of mappings' which transforms the variable (unknown) domain to a fixed region by means of a suitable mapping. The given problem then turns into a parameter estimation problem to determine the coefficients of an elliptic problem on a fixed domain (cf. Banks et al. [9],[10] for parabolic equations).

2. DIRECT PROBLEM

Consider a bounded domain $G(q) \subset \mathbb{R}^2$ defined by

$$G(q) = \{(x, y) \in \mathbb{R}^2 | 0 < x < 1, 0 < y < r(x, q)\}$$

where $r(x,q) \in C[0,1]$, $q \in Q$ characterizes the shape of a part of the boundary, which depends on the constant parameterization vector $q \in Q$. Here, Q is a given compact set in \mathbb{R}^n , $n \in \mathbb{N}$. It is obvious, that the boundary of G(q)consists of the following components:

$$\begin{split} \Sigma_1 &= \{(x,y)| \quad 0 < x < 1, \ y = 0\} \\ \Sigma_2 &= \{(x,y)| \quad x = 0, \ 0 < y < r(0,q)\} \\ \Sigma_3 &= \{(x,y)| \quad x = 1, \ 0 < y < r(1,q)\} \\ \Sigma_q &= \{(x,y)| \quad 0 < x < 1, \ y = r(x,q)\} \end{split}$$

In this geometric setting we consider the following direct problem (see Fig.??) : Given the parameter vector $q \in Q$, find a function u, such that

$$-\Delta u = 0 \quad \text{in } G(q) \tag{1}$$

with the mixed boundary conditions

$$\frac{\partial u}{\partial \nu} = g_1 \quad \text{on } \Sigma_1 \tag{2}$$

$$\frac{\partial u}{\partial \nu} = g_2 \quad \text{on } \Sigma_2 \tag{3}$$

$$\frac{\partial u}{\partial \nu} = g_3 \quad \text{on } \Sigma_3 \tag{4}$$

$$u = f_q \quad \text{on } \Sigma_q \,, \tag{5}$$

where $g_i \in L_2(\Sigma_i)$, i = 1, 2, 3, $f_q \in L_2(\Sigma_q)$ and ν denotes the outer unit normal to $\partial G(q)$.

If we define the function sets

$$\begin{split} &H^{1}_{f_{q}|\Sigma_{q}}(G_{q}) &:= \{ u \in H^{1}(G_{q}) | \quad u | \Sigma_{q} = f_{q} \} \\ &H^{1}_{0|\Sigma_{q}}(G_{q}) &:= \{ u \in H^{1}(G_{q}) | \quad u | \Sigma_{q} = 0 \} \end{split}$$

a weak formulation of the problem can also be given: Find a function $u \in H^1_{f_q|\Sigma_q}(G_q)$, such that:

$$(\nabla u, \nabla v)_{L_2(G_q)} = (g, v)_{L_2(\overline{\Sigma})} \quad \forall v \in H^1_{0|\Sigma_q}(G_q), \ (6)$$

where $\overline{\Sigma} := \Sigma_1 \cup \Sigma_2 \cup \Sigma_3$, $g := g_i$ on Σ_i , i = 1, 2, 3. For questions concerning the existence and uniqueness of solutions to this direct problem, we refer to [11],[12],[13].



3. INVERSE PROBLEM

If the parameter vector q is unknown, and Σ_q has to be identified, the inverse problem can be posed as follows (see Fig. ??): Given additional Dirichlet data $u = f_1^{\varepsilon}$ on Σ_1 , find a pair (u, q), resp. (u, G(q)), such that u solves the direct problem (1)-(5). The notation f_1^{ε} reminds to the fact, that the true data f_1 may be perturbed by a random error of maximum amount ε . It is known, that such problems are ill-posed (cf. [14]), so we have to take into consideration, that small data errors can cause large errors in the solution.



4. NUMERICAL METHOD

One possibility to deal with such boundary identification problems is the so called "method of mappings" (see [2],[9],[10]). Roughly speaking, the fixed BVP on a variable domain is transformed into a BVP with variable coefficients on a fixed reference domain and then this coefficient identification problem has to be solved.

Our approach to the problem is a different one, namely to solve the minimization problem: Find $\hat{q} \in Q$, which satisfies

$$J(\hat{q}) = \min_{q \in Q} J(q) \,,$$

where the minimized "defect-functional" J(q) is given by

$$J(q) = \|u(q)|\Sigma_1 - f_1^{\varepsilon}\|_{L_2(\Sigma_1)}^2 , \quad q \in Q$$

and u(q) solves the direct problem on G(q). As a minimization method we make use of the Gradient Projection Method for nonlinear optimization problems with linear constraints as it is described in [16], [17]. To be more precise the steps of our method are as follows:

- 1. Determine an initial guess $q^{(0)} \in Q \setminus \partial Q$ as a starting point. Set $q^{(1)} := q^{(0)}$, and set the set H of active constraints to $H := \emptyset$.
- 2. Compute an approximation to $-\nabla_q J(q)(q^{(1)})$. For this purpose, we use a forward differences of first order (with a suitable chosen step length), so we have to solve three direct problems in this step. If $\nabla_q J(q)(q^{(1)}) = 0$, which means that $q^{(1)}$ is a stationary point, terminate the computation with the result $q^{(1)}$.
- 3. If $q^{(1)}$ is an inner point of Q the current direction is defined by the unit vector

$$d := \frac{-\nabla_q J(q)(q^{(1)})}{\|\nabla_q J(q)(q^{(1)})\|}$$

and we continue with step 5. If $q^{(1)}$ is on ∂Q , d is set to be the projection of

$$\frac{-\nabla_q J(q)(q^{(1)})}{\|\nabla_q J(q)(q^{(1)})\|}$$

onto H, and if $d \neq 0$ we continue with step 5, else we continue with step 4.

4. Compute the vector $\theta(q^{(1)})$ by

$$\theta(q^{(1)}) = (\Pi \Pi^T)^{-1} \Pi \nabla_q J(q)(q^{(1)}),$$

where the columns of Π consist of the normal vectors of the active constraints in H. If all components of $\theta(q^{(1)})$ are non-positive, then terminate the computation with the result $q^{(1)}$, else drop the constraint in H (and in Π) corresponding to the maximum value in $\theta(q^{(1)})$. Then return to step. 3

5. Determine λ_m , which is the largest step to be taken in direction d without violating any (non-active) constraint, compute λ_0 as the solution of

$$\lambda_0 = \min_{\lambda \in [0,\lambda_m]} J(q^{(1)} + \lambda d)$$

and set $q^{(1)} := q^{(1)} + \lambda_0 d$. If $\lambda_0 = \lambda_m$ then add the new constraint to H (resp. a new column to Π).

6. If an additional stopping criterion (like a certain number of iterations or a defined grade of accuracy) is fulfilled, stop the computation, else return to step 2. (This step is needed, since we cannot expect the functional J(q) to be convex on Q, so we cannot be sure that the algorithm will converge resp. stop.)

5. COMPUTATIONAL RESULTS

In our numerical examples we focuse on a special case for the set Q. We assume the shape of the unknown boundary to be a straight line, i.e.

$$r(x,q) := q_1 + q_2 x$$

with the compact set Q given by

$$Q := \{ (q_1, q_2) \in \mathbb{R}^2 | 0.5 \le q_1 \le 5, \, 0 \le q_2 \le 5 \}$$

We chose

$$\hat{q}_0 = \hat{q}_1 = 2$$

as parameters describing the true boundary $\Sigma_{\hat{q}}$ and compute solutions of two different direct problems. In the first example we choose

$$f_q^1 = 10$$

$$g_1 = 1$$

$$g_2 = g_3 = -1$$

and in the second one we change f_q to $f_q^2(x) = 10x$, $x \in [0,1]$ keeping the values for g_i , i = 1, 2, 3. We use standard finite-element methods for elliptic problems to solve these problems with a discretization parameter h = 0.1, and we denote the computed solutions by u^1 , u^2 belonging to f_q^1 , f_q^2 , resp. . The next step is to define our "data" by

$$f_1^{\varepsilon,j} := u^j | \Sigma_1 + \varepsilon \cdot \text{random} , j = 1, 2, \text{ random} \in [-1, 1]$$

In all experiments we chose $\varepsilon = 10^{-2}$. In addition to the Gradient Projection Method (GPM), which we described in the preceding section, we made use of another method

for nonlinear optimization to minimize the functional J(q), namely the Nelder-Mead Simplex Method (NMSM) (see [15] and the references therein). It turned out, that both methods provided comparable results. One cannot expect the functional J(q) to be convex and twice continuously differentiable – in this case at least the GPM would converge to the absolute minimum [16] (for the convergence properties of the NMSM see [15],[18]).Therefore we have chosen different starting points in our numerical experiments. In our results we can very well observe the fact, that the problem is ill-posed, namely, for a pair of data $\sigma_{1,ex.}$, $\sigma_{1,app.}$ on Σ_1 with

$$\|\sigma_{1,ex.} - \sigma_{1,app.}\|_{L_2(\Sigma_1)} \le 10^{-3}$$

the corresponding values of q were $\hat{q} = (2,2)$, $q_{app.} = (1.72, 3.56)$). We also found, that the boundary condition on Σ_q influences the possibilities to identify the parameters (q_1, q_2) . Therefore we will discuss the results for the two examples for f_q in the following paragraph.

5.1 Results for $f_q = f_q^1 = 10$

In this case the identification of q_1 seems to be much easier than the identification of q_2 . From none of the starting points the relative error concerning q_1 was bigger than 7.5% (for the GPM) resp. 3.5% (for the NMSM) after the minimization procedure (see Table 1). In contrast the computed values for q_2 seem to depend very much on the starting point, and the relative error for this parameter is much larger than for q_1 . This means that the value r(x,0) is computed relatively exact, while the slope of the unknown boundary can only be roughly estimated by our computations (cf. Fig. 1). The reason for this becomes clear, if we look at the shape of the functional J(q) in this case (see Figure 2). Due to the steep gradients in the q_1 -direction we find relatively easy, that q_1 must lie near the value 2. But as the figure suggests, it is much more difficult to minimize J(q) along $q_1 = 2$, and we observe that there are a lot of local minimizers (for all starting points in Table 1 the value of J(q) after the minimization procedure was less than 10^{-5} .

Because there is no significant change of the computed solution q as well as of the value of J(q) after about four or five steps of the GPM, we stopped the computation at this point. Of course one could also apply other stopping criteria like the Morozov and the Nemirowskii stopping rule.

5.2 Results for $f_{\rm q}=f_{\rm q}^2=10 {\rm x}$

With the modified boundary condition on Σ_q we get computational results which differ from those in Section 5.1 in some aspects. Figure 3 shows certain characteristic features of our results: The approximation to q_1 is not as exact as in Section 5.1, but in most cases we get a slightly better approximation to q_2 than before. Motivated by the results for different starting points (see. Table 2 and Figure 4) we might assume that there is – as before – a strip in the (q_1, q_2) -plane, where the local minimizers are located. Now there is no strip parallel to any of the axes, but taking into account Figure 4 it might (purely heuristically) be described by an appropriate neighbourhood of the line

$$q_1 + 2q_2 = 6$$

It is an interesting task for further examinations, to clarify the relationship between the location of the local minimizers and the boundary condition on Σ_q .

6. NOMENCLATURE

d		unit vector in GPM (current direction)
f_1		data corresponding to the
		true solution \hat{q}
f_1^{ε}		perturbed data
f_q		function describing the Dirichlet-
		condition on Σ_q
g_1		Neumann-condition on Σ_1
g_2		Neumann-condition on Σ_2
g_3		Neumann-condition on Σ_3
G(q)	=	$\{(x, y) \in \mathbb{R}^2 0 < x < 1, 0 < y < r(x, q)\}$
		bounded domain
BVP		boundary value problem
Н		set of active constraints
$H^1_{f_q \Sigma_q}(G_q)$	=	$\{u \in H^1(G_q) u \Sigma_q = f_q\}$
$H^1_{0 \Sigma_q}(G_q)$	=	$\{u\in H^1(G_q) u \Sigma_q=0\}$
J(q)	=	$ u(q) \Sigma_1 - f_1 ^2_{L_2(\Sigma_1)}$
$n \in \mathbb{N}$		dimension of parameter vector
Q		compact subset of \mathbb{R}^n
q	=	$(q_1,\ldots,q_n) \in Q$ parameter vector,
		on which $r(x,q)$ depends
\hat{q}		true parameter vector
r(x,q)	\in	$C[0,1] \forall q \in Q \text{shape of the}$
		unknown part of the boundary
ε		maximum amount of data perturbation
ν		the outer unit normal to $\partial G(q)$
Σ_1	=	$\{(x,y) 0 < x < 1, y = 0\}$
Σ_2	=	$\{(x,y) x = 0, 0 < y < r(0,q) \}$
Σ_3	=	$\{(x,y) x=1, 0 < y < r(1,q)\}$
Σ_q	=	$\{(x,y) 0 < x < 1, \ y = r(x,q)\}$
Σ	=	$\Sigma_1 \cup \Sigma_2 \cup \Sigma_3$
Π		Matrix of normal unit vectors
		of active constraints ∂ ∂
$ abla_q$	=	$\left(\frac{\partial}{\partial q_1},\ldots,\frac{\partial}{\partial q_n}\right)$
\forall		for all

7. REFERENCES

- 1. O. Pironneau, Optimal shape design for elliptic systems, Springer, New York, 1984.
- 2. D. D. Ang, L. K. Vy, Domain identification for harmonic functions, Act. App. Math., vol. 38, pp. 217-238,1995

- 3. G. Alessandrini, L. Rondi, Stable determination of a crack in a planar inhomogenous conductor, SIAM J. Math. Anal., vol. 30, pp. 326-340, 1998.
- 4. V. Isakov, New stability results for soft obstacles in inverse scattering, Inverse Problems, vol. 9, pp. 535-543, 1993.
- 5. P. G. Kaup, F. Santosa, M. Vogelius, Method for imaging corrosion damage in thin plates from electrostatic data, Inverse Problems, vol. 12, pp. 279-293, 1996.
- 6. Dinh Nho Hào, H.-J. Reinhardt, Gradient methods for inverse heat conduction problems, Inverse Prob*lems in Engineering*, vol. 6, pp. 177-211, 1998.
- 7. V. A. Morozov, Methods for Solving Incorrectly Posed Problems, Springer, New York, 1984.
- 8. A. S. Nemirovskii, The regularizing properties of the adjoint gradient method in ill-posed problems, U. S. S. R. Comput. Math. Math. Phys., vol. 26, pp. 7-16, 1986.
- 9. H. T. Banks, F. Kojima, Boundary shape identification problems in two-dimensional domains related to thermal testing of materials, Quarterly of applied mathematics, vol. 47, no.2, pp. 273-293, 1989.
- 10. H. T. Banks, F. Kojima, Boundary estimation arising in thermal tomography, Inverse Problems, vol. 6, pp. 897-921, 1990.
- 11. P. Grisvard, Elliptic problems in nonsmooth domains, Pitman, Boston, 1985.
- 12. D. Gilbarg, N.S. Trudinger, Elliptic partial differential equations of second order, Springer, New York, 1977.
- 13. J. L. Lions, E. Magenes, Non-homogenous boundary value problems and applications, Springer, New York, 1972.
- 14. G. Alessandrini, Examples of instability in inverse boundary value problems, Inverse Problems, vol. 13, pp. 887-897, 1997.
- 15. J. C. Lagarias, J. A. Reeds, M. H. Wright, P. E. Wright, Convergence properties of the Nelder-Mead simplex method in low dimensions, SIAM Journal of Optimization, vol. 9, no. 1, pp. 112-147, 1998.
- 16. J. B. Rosen, The gradient projection method for nonlinear programming. Part I. Linear constraints, J. Soc. Indust. Appl. Math., vol. 8, no. 1, pp. 181-217, 1960.
- 17. E. Polak, Computational methods in optimization, Academic Press, New York, 1971.
- 18. K. I. M. McKinnon, Convergence of the Nelder-Mead simplex method to a nonstationary point, SIAM Journal of Optimization, vol.9, no. 1, pp. 148-158, 1998.



Figure 1: True solution and approximations for $f_q = 10$ with starting point (3,3)



Figure 2: The functional J(q) for $f_q = 10$



Figure 3: True solution and approximations for $f_q = 10x$ with starting point (1,1)



Figure 4: The functional J(q) for $f_q = 10x$