

## Regularized Parameter Identification in Elliptic Boundary Value Problems<sup>1)</sup>

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In der Arbeit wird die Methode der Regularisierung zur numerischen Identifikation des Diffusionskoeffizienten in elliptischen Gleichungen zweiter Ordnung untersucht. Zur Lösung der entsprechenden regularisierten diskreten und stetigen Minimierungsaufgaben wird das Gauß-Newton-Verfahren analysiert. Es wird ein effektiver Weg beschrieben, der pro Iterationsschritt das Lösen einer Gleichung zweiter Ordnung und einer Gleichung vierter Ordnung erfordert.

В работе исследуются методы регуляризации численной идентификации коэффициента диффузии эллиптического уравнения второго порядка. Обсуждается применение метода Гаусса-Ньютона для решения соответствующих регуляризованных дискретных и непрерывных экстремальных задач. Описывается эффективный алгоритм, требующий решения одного уравнения второго порядка и одного уравнения четвертого порядка на каждой итерации.

In this paper the regularization method applied to the numerical identification of the diffusion coefficient in second order elliptic equations is investigated. For solving the corresponding regularized discrete and continuous nonlinear minimization problems the Gauss-Newton method is analyzed. We describe an effective way for performing one iteration step which requires to solve one problem of 2nd order and one problem of 4th order.

### 1. Introduction

In this paper we investigate parameter identification problems and their approximations for a special class of elliptic boundary value problems. Although our ideas are applicable to a wide class of identification problems, our work here is devoted to a special inverse problem of aquifer transmissivity identification (cf. [1, 27]). As our fundamental state equation we consider the elliptic equation

$$-\operatorname{div}(a \operatorname{grad} u) = f, \quad x \in \Omega. \quad (1.1)$$

This equation, for example, describes the steady flow in a confined nonuniform aquifer  $\Omega$ , where  $a = a(x)$  denotes the spatially varying transmissivity coefficient of the aquifer,  $u = u(x)$  the (observed) piezometric head and  $f \cong f(x)$  the source term. In the direct problem for given  $a$ ,  $f$  and appropriate boundary conditions the unique solution  $u$  is to be determined. This direct problem, in general, is a well-posed one.

In the parameter identification problem  $a$  is to be found for given  $u$  and  $f$ . In this problem we are faced with the identifiability problem and with a noncontinuous dependence of  $a$  on the observation data  $z = u + \eta$  ( $\eta$  denotes the observation error) with respect to any meaningful observation topology. We say  $a$  is *identifiable* if, for given  $u$  and  $f$  and given boundary conditions,  $a$  is unique. Several authors (cf. [4, 6, 22]) study the identifiability of  $a$  in one- and higher-dimensional problems (1.1) and

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the paper [18] investigates the identifiability of  $a$  in different discretized versions of (1.1) for one space dimension. The noncontinuous dependence of  $a$  from  $z$  is caused by the differentiation of  $z$  in order to determine  $\text{grad } u$  and can lead to serious difficulties if the infinite-dimensional identification problem is approximated by finite-dimensional problems. The numerical solution may show undesirable oscillations or may not converge at all. Therefore, special identification techniques are needed to overcome such difficulties. The accompanying is a partial list of numerical methods for parameter identification:

1. Least Squares Methods [3, 5, 6, 18],
2. Tichonov's Regularization Methods [9, 16, 21, 24],
3. Adaptive (or Asymptotic) Regularization Methods [2, 12].

All these methods use further a priori information about the parameter to be determined in order to overcome the ill-posedness of the identification problem.

The present paper is organized as follows. In Section 2 we describe the Tichonov's regularization method for parameter identification problems and its Galerkin approximations. Section 3 contains results to the effective numerical solution of the corresponding discrete nonlinear minimization problems by the Gauss-Newton method. In Section 4 we generalize the results of Section 3 to the continuous case and show that one iteration step of the Gauss-Newton method requires only to solve one problem of 2nd order and one problem of 4th order.

## 2. Parameter identification by Tichonov's regularization

As our fundamental state equation which is used in the sequel we consider the following prototype of a two point boundary value problem

$$-(au_x)_x = f, \quad x \in (0, 1), \quad (2.1)$$

with any of the three boundary conditions:

$$u(0) = g_0, u(1) = g_1, \quad (2.2)$$

$$a(0) u_x(0) = g_0, a(1) u_x(1) = g_1, \quad (2.3)$$

$$a(0) u_x(0) + s_0 u(0) = g_0, a(1) u_x(1) + s_1 u(1) = g_1. \quad (2.4)$$

The function  $a$  is supposed to be unknown so we shall consider the problem of identifying the function from observations of the state variable  $u$ . This problem is ill-posed. Let us consider a specific case in which continuity of  $a$  with respect to  $u$  is violated. Consider (2.1), (2.2) with  $f = 0$ ,  $g_0 = 1$ ,  $g_1 = 2$  and  $a(0) = 1$ . Given the data  $u(x) = 1 + x$ , then (2.1) has the unique solution  $a(x) = 1$ . Given the data  $u_k(x) = u(x) + \sin 2k\pi x / (2k\pi)$ , then (2.1) has the unique solution  $a_k(x) = 3 / (2 + \cos 2k\pi x)$ . Then obviously,  $u_k$  converges to  $u$  uniformly with increasing  $k$ , whereas for all  $k$ ,

$$\begin{aligned} \|a - a_k\|_{L^2(0,1)}^2 &= \int_0^1 \frac{(1 - \cos 2k\pi x)^2}{(2 + \cos 2k\pi x)^2} dx \\ &= \left[ x - \frac{3}{2k\pi} \frac{\sin 2k\pi x}{2 + \cos 2k\pi x} \right]_0^1 = 1. \end{aligned}$$

In summary,  $u_k \rightarrow u$ , yet  $a_k \not\rightarrow a$  and  $a$  is therefore not a continuous function of the data.

The state equations (2.1) with any of the three boundary conditions (2.2)–(2.4) (in case (2.2) for simplicity we suppose homogeneous boundary conditions) can be written in weak formulation:

$$\langle au_x, v_x \rangle = \langle f, v \rangle \quad \forall v \in U, \quad (2.5)$$

$$\langle au_x, v_x \rangle = \langle f, v \rangle + g_1 v(1) - g_0 v(0) \quad \forall v \in U, \quad (2.6)$$

$$\langle au_x, v_x \rangle + s_1 u(1) v(1) - s_0 u(0) v(0) = \langle f, v \rangle + g_1 v(1) - g_0 v(0) \quad \forall v \in U \quad (2.7)$$

( $\langle \cdot, \cdot \rangle$  denotes the scalar product of  $L^2(0, 1)$ ). Choosing  $A = H^1(0, 1)$ ,  $f \in L^2(0, 1)$ ,  $A_c = \{a \in A : a(x) \geq a \text{ a.e. } x \in (0, 1), \text{ for some } a > 0\}$ , then the following results with respect to solvability of the variational equations (2.5)–(2.7) are valid (cf. [28]).

Lemma 1: For any  $a \in A_c$ , the following is true:

(i) there exists a unique solution  $u \in U = H_0^1(0, 1)$  to (2.5);

(ii) under the condition  $\int_0^1 f dx + g_1 - g_0 = 0$  there exists a unique solution  $u \in U_c = \left\{ u \in U = H^1(0, 1) : \int_0^1 (u - z) dx = 0 \right\}$  to (2.6);

(iii) under the conditions  $s_0 < 0 < s_1$  there exists a unique solution  $u \in U = H^1(0, 1)$  to (2.7).

Remark: In fact, a stronger result is possible, i.e. Lemma 1 remains true for any  $a \in A_c = \{a \in L^\infty(0, 1) : a(x) \geq a \text{ a.e. } x \in (0, 1); \text{ for some } a > 0\}$ .

Let us introduce the set  $A_{ad} \subset A_c$  of physically admissible parameters  $a$  and let  $b \in A_{ad}$  a suitable estimate of the unknown parameter  $a$ . Furthermore, for a brief notation let us rewrite the problems (2.5)–(2.7) in form of an operator equation

$$\mathfrak{F}(a, u) = \varphi, \quad (2.8)$$

where the bilinear operator  $\mathfrak{F} : A_c \times U \rightarrow U^*$  induced by the left-hand sides of (2.5)–(2.7) is bounded. Applying Tichonov's regularization method (cf. [25]) to the identification problem we are led to the nonlinear programming problem

$$(P) \quad \inf_{a \in A_{ad}} J_\alpha(a); \quad J_\alpha(a) = \frac{1}{2} \|u - z\|_{L^2(0, 1)}^2 + \frac{\alpha}{2} \|a - b\|_{L^2(0, 1)}^2,$$

where  $u(x; a)$  satisfies (2.8).

Here  $\alpha > 0$  denotes the regularization parameter to be chosen appropriately (cf. [13]). Roughly speaking, the term  $\|a - b\|_{L^2(0, 1)}^2$  in the functional  $J_\alpha$  prevents the solution  $a$  from the divergence. We now consider the approximation of problem (P). In the following we describe a Galerkin-based parameter/state approximation scheme in the same spirit of the ideas found in [18] and divide our considerations into two stages. In the first stage we carry out the parameter approximation. That is, we seek the parameters  $\hat{a}$  in the form  $a^m = a_1 \varphi_1 + \dots + a_m \varphi_m$ , where  $A_m = \mathfrak{L}(\varphi_1, \varphi_2, \dots, \varphi_m)$  denotes an  $m$ -dimensional subspace of  $A := \mathfrak{L}(\varphi_1, \varphi_2, \dots, \varphi_m; \varphi_{m+1}, \dots)$  and describe this approximation by the bounded linear projection operator  $\mathfrak{B}^m : A \rightarrow \mathbf{R}^m$ ,  $\mathfrak{B}^m a := \hat{a}$  if  $\hat{a} = a^m$ ,  $\mathfrak{B}^m \varphi_i := 0$  if  $i > m$  with  $\hat{a} = (a_1, a_2, \dots, a_m)^T \in \mathbf{R}^m$ . Introducing the finite-dimensional set  $A_{ad}^m = \mathfrak{B}^m A_{ad}$ , we are led to the parameter approxi-

mation problem

$$(P_m) \quad \min_{\bar{a} \in A_{\bar{a}}^m} J_a(\bar{a}); \quad J_a(\bar{a}) = \frac{1}{2} \|u - z\|_{L^2(0,1)}^2 + \frac{\alpha}{2} \|\bar{a} - \mathfrak{B}^m b\|_{\mathbb{R}^m}^2,$$

where  $u(x; a^m)$  satisfies (2.8).

In the second stage we consider the approximation of the state equations (2.5)–(2.7). That is, we seek approximate solutions to (2.5)–(2.7) in the form  $u^n = u_1 \psi_1 + \dots + u_n \psi_n$ , where  $U_n = \mathfrak{L}(\psi_1, \psi_2, \dots, \psi_n)$  denotes an  $n$ -dimensional subspace of  $U = \mathfrak{L}(\psi_1, \psi_2, \dots; \psi_n, \psi_{n+1}, \dots)$  and describe this approximation by the bounded linear projection operator  $\mathfrak{Q}^n: U \rightarrow \mathbb{R}^n$ ,  $\mathfrak{Q}^n u := \bar{u}$  if  $u = u^n$ ,  $\mathfrak{Q}^n \psi_i := 0$  if  $i > n$  with  $\bar{u} = (u_1, u_2, \dots, u_n)^T \in \mathbb{R}^n$ . Introducing the differentiation operator  $D = d/dx$  the corresponding state equations (2.5)–(2.7) can be approximated by ( $i = 1, 2, \dots, n$ )

$$\langle a^m D u^n, D \psi_i \rangle = \langle f, \psi_i \rangle, \quad (2.9)$$

$$\langle a^m D u^n, D \psi_i \rangle = \langle f, \psi_i \rangle + g_1 \psi_i(1) - g_0 \psi_i(0), \quad (2.10)$$

$$\langle a^m D u^n, D \psi_i \rangle + s_1 \dot{u}^n(1) \psi_i(1) - s_0 u^n(0) \psi_i(0) = \langle f, \psi_i \rangle + g_1 \psi_i(1) - g_0 \psi_i(0). \quad (2.11)$$

Note that these approximated state equations can be written in the compact form

$$F(\bar{a}, \bar{u}) = \bar{f}, \quad F: (\bar{a}, \bar{u}) \in \mathbb{R}^m \times \mathbb{R}^n \rightarrow \mathbb{R}^n. \quad (2.12)$$

Let us regard a special example. Let  $(0, 1)$  be partitioned into  $N$  subintervals of length  $h = 1/N$ . For  $i = 1, \dots, N$  we define the 0th order spline basis functions

$$\varphi_i(x) = \begin{cases} 1, & (i-1)h \leq x \leq ih, \\ 0, & \text{otherwise} \end{cases}$$

and for  $j = 1, \dots, N-1$  the linear spline basis functions

$$\psi_j(x) = \begin{cases} Nx + 1 - j, & (j-1)h \leq x \leq jh, \\ -Nx + 1 + j, & jh \leq x \leq (j+1)h, \\ 0, & \text{otherwise.} \end{cases}$$

Thus we have chosen  $m = N$  and  $n = N-1$ . Let us regard the approximate state equation (2.9). Then it is straightforward to compute analytically the integrals of the system (2.9) and hence to obtain the corresponding parametric finite-dimensional operator equation (2.12) in the form

$$-a_{i+1}(u_{i+1} - u_i) + a_i(u_i - u_{i-1}) = h^2 \langle f, \psi_i \rangle, \quad i = 1, \dots, N-1, \quad (2.13)$$

where  $u_0 = u_N = 0$ .

Now we are able to formulate the parameter/state approximation problem:

$$(P_{m,n}) \quad \min_{\bar{a} \in A_{\bar{a}}^m} J_a(\bar{a}); \quad J_a(\bar{a}) = \frac{1}{2} \|\bar{u} - \mathfrak{Q}^n z\|_{\mathbb{R}^n}^2 + \frac{\alpha}{2} \|\bar{a} - \mathfrak{B}^m b\|_{\mathbb{R}^m}^2,$$

where  $\bar{u}$  satisfies (2.12).

### 3. Solution of the discrete minimization problems

In this chapter we examine the numerical solution of problem  $(P_{m,n})$ , which is a finite-dimensional nonlinear programming problem to obtain the coefficients  $a_1, a_2, \dots, a_m$  of the unknown function  $a^m(x) = a_1 \varphi_1(x) + \dots + a_m \varphi_m(x)$ . One possibility for

solving this nonlinear programming problem is to use a gradient projection method. The main work required at each iteration is to evaluate the gradient  $(\partial J_a(\bar{a})/\partial a_1, \dots, \partial J_a(\bar{a})/\partial a_m)^T$ . This can be done after introducing of an appropriate adjoint variable by the solution of only two linear systems of equations with a sparse matrix (cf. [3, 24]). Since problems  $(P_{m,n})$  in general have a flat global minimum in deep banana shaped valleys, they should better be treated by (projected) Gauss-Newton methods which make it possible to proceed in great steps along the deep valleys and assures fast convergence. Let  $\widetilde{\Delta u}[\widetilde{\Delta a}]$  be the solution of the linearized finite-dimensional state equation

$$F_{\bar{u}}' \widetilde{\Delta u} + F_{\bar{a}}' \widetilde{\Delta a} = 0 \tag{3.1}$$

where  $F_{\bar{u}}' = F_{\bar{u}}'(\bar{a}, \bar{u})$  and  $F_{\bar{a}}' = F_{\bar{a}}'(\bar{a}, \bar{u})$  denote the Frechet derivatives of the mapping  $F$  with respect to  $\bar{u}$  and  $\bar{a}$ . Then in the (projected) Gauss-Newton method a given approximation  $\bar{a} \in \mathbb{R}^m$  is improved by

$$\bar{a} := P_{ad}^m[\bar{a} + \gamma \widetilde{\Delta a}], \tag{3.2}$$

where  $\widetilde{\Delta a}$  is the solution of the linearized problem

$$(P_{m,\bar{a}}^1) \quad \inf J_a^1(\widetilde{\Delta a}); J_a^1(\widetilde{\Delta a}) = \frac{1}{2} \|\bar{u} + \widetilde{\Delta u}[\widetilde{\Delta a}] - \Omega^n z\|_{\mathbb{R}^n}^2 + \frac{\alpha}{2} \|\bar{a} + \widetilde{\Delta a} - \mathfrak{P}^m b\|_{\mathbb{R}^m}^2,$$

where  $\widetilde{\Delta u}[\widetilde{\Delta a}]$  satisfies (3.1),

$P_{ad}^m$  is the projection onto  $A_{ad}^m$  and  $\gamma$  is the steplength parameter to be chosen appropriately (cf. [23]). At first glance, method (3.2) seems to be rather expensive compared with gradient projection methods. Fortunately we have found a route how the amount of computational work in solving  $(P_{m,n}^1)$  can be reduced substantially compared with traditional strategies.

**Theorem 1:** *Let  $F_{\bar{u}}'$  be a regular matrix. Then problem  $(P_{m,n}^1)$  is uniquely solvable. The unique solution  $\widetilde{\Delta a} \in \mathbb{R}^m$  is given by*

$$\widetilde{\Delta a} = \mathfrak{P}^m \bar{b} - \bar{a} + F_{\bar{a}}'^* \bar{q}, \tag{3.3}$$

where  $\bar{u} \in \mathbb{R}^n$  is the unique solution of (2.12) and  $\bar{q} \in \mathbb{R}^n$  is the unique solution of

$$(F_{\bar{a}}' F_{\bar{a}}'^* + \alpha F_{\bar{u}}' F_{\bar{u}}'^*) \bar{q} = F_{\bar{a}}'(\bar{a} - \mathfrak{P}^m b) + F_{\bar{u}}'(\bar{u} - \Omega^n z). \tag{3.4}$$

**Proof:** The existence and uniqueness of  $\widetilde{\Delta a}$  follows from the fact that

$$\partial^2 J_a^1(\widetilde{\Delta a})/\partial \widetilde{\Delta a}^2 = F_{\bar{a}}'^*(F_{\bar{u}}' F_{\bar{u}}'^*)^{-1} F_{\bar{a}}' + \alpha I$$

is positive definite. Now let us regard

$$J_a^1(\widetilde{\Delta a} + t\bar{v}) = \frac{1}{2} \|\widetilde{\Delta u}[\widetilde{\Delta a} + t\bar{v}] + \bar{u} - \Omega^n z\|_{\mathbb{R}^n}^2 + \frac{\alpha}{2} \|\bar{a} + \widetilde{\Delta a} + t\bar{v} - \mathfrak{P}^m b\|_{\mathbb{R}^m}^2.$$

Differentiation with respect to  $t$  yields for all  $\bar{v} \in \mathbb{R}^m$

$$\frac{\partial}{\partial t} J_a^1(\widetilde{\Delta a} + t\bar{v})|_{t=0} = (\widetilde{\Delta u}[\widetilde{\Delta a}] + \bar{u} - \Omega^n z, \widetilde{\Delta u}[\bar{v}]) + \alpha(\bar{a} + \widetilde{\Delta a} - \mathfrak{P}^m b, \bar{v}) = 0 \tag{3.5}$$



where  $\Delta u[w]$ ,  $w \in L^\infty(0, 1)$ , solves one of the linear variational problems

$$\left. \begin{aligned} \langle a \Delta u_x, v_x \rangle &= -\langle w u_x, v_x \rangle & \forall v \in U = H_0^1(0, 1), \\ \langle a \Delta u_x, v_x \rangle &= -\langle w u_x, v_x \rangle & \forall v \in U = H^1(0, 1), \\ \langle a \Delta u_x, v_x \rangle + s_1 \Delta u(1) v(1) - s_0 \Delta u(0) v(0) &= -\langle w u_x, v_x \rangle & \forall v \in U = H^1(0, 1) \end{aligned} \right\} \quad (4.2)$$

according to the corresponding boundary conditions (2.2)–(2.4). These second order equations we consider in an  $H^{-1}$ -weak formulation. That means the set of test functions  $v$  will be reduced to allow a further partial integration on the left-hand side. After defining the space of test functions

$$V = \left\{ v: av_x \in H^1, \begin{cases} v(0) = 0, v(1) = 0 \text{ or} \\ v_x(0) = 0, v_x(1) = 0 \text{ or} \\ a(0)v_x(0) + s_0 v(0) = 0, a(1)v_x(1) + s_1 v(1) = 0 \end{cases} \right\} \quad (4.3)$$

we get the  $H^{-1}$ -weak formulation for the problem (4.2)

$$\langle \Delta u, (av_x)_x \rangle = \langle w u_x, v_x \rangle = \langle w, u_x v_x \rangle \quad \forall v \in V \quad (4.4)$$

for all the three cases of boundary conditions. Note that in this formulation the supposition  $w \in L^\infty(0, 1)$  can be weakened to  $w \in L^2(0, 1)$ . Analogously to Theorem 1 we have

**Theorem 2:** *Let be  $a \in L^\infty(0, 1)$  with  $a(x) \geq \underline{a} > 0$ . There exists one and only one element  $\Delta a^* \in L^2(0, 1)$ , which minimizes the linearized functional (4.1). This element  $\Delta a^*$  can be characterized by the weak solution  $q \in V$  of the 4th order equation*

$$\langle u_x q_x - (a - b), u_x v_x \rangle + \langle u - z + \alpha(aq_x)_x, (av_x)_x \rangle = 0 \quad \forall v \in V \quad (4.5)$$

by

$$\Delta a^* = u_x q_x - (a - b). \quad (4.6)$$

Note that the equation (4.5) is the continuous analogue to the discrete problem (3.4).

**Proof:** The minimizing element  $\Delta a^*$  has to fulfil the necessary and sufficient minimum condition for the quadratic functional (P<sup>1</sup>)

$$\langle \Delta u[\Delta a^*] + u - z, \Delta u[r] \rangle + \alpha \langle \Delta a^* + a - b, r \rangle = 0 \quad \forall r \in L^2(0, 1). \quad (4.7)$$

Let  $q$  be a solution of the equation (4.5). The equation (4.5), (4.6) together with (4.4) gives us an  $H^{-1}$ -weak solution

$$\Delta u[\Delta a^*] = -\{u, -z + \alpha(aq_x)_x\}. \quad (4.8)$$

Rewriting the  $H^{-1}$ -weak formulation (4.4) for  $\Delta u[r]$  with  $q \in V$  instead of an arbitrary  $v \in V$ , we get  $\langle \Delta u[r], (aq_x)_x \rangle = \langle r, u_x q_x \rangle$ . This relation together with (4.8) and (4.6) shows, that the minimum condition (4.7) holds for all  $r \in L^2(0, 1)$  ■

Due to the well-posedness of (4.5) for fixed  $\alpha > 0$  there is no fear of ill-conditioning in the discrete problem (3.4) for decreasing stepsizes.

**Remarks:** 1. Theorem 2 deals only with the case  $\Delta a^* \in L^2(0, 1)$ . The representation (4.6) shows that  $u_x$  is the decisive quantity for  $\Delta a^*$  being an element of  $L^\infty(0, 1)$ . In order to get  $u_x \in L^\infty(0, 1)$  we need some not too hard additional assumptions on  $f \in H^{-1}(0, 1)$  for the problem (2.1) (for instance,  $f \in L^2(0, 1)$  gives  $u_x \in L^\infty(0, 1)$ ). 2. If we formally perform (4.5)

by partial integration we get the 4th order equation

$$\alpha(a(aq_x)_{xx})_x - (u_x^2 q_x)_x = (a(z - u)_x)_x - ((a - b) u_x)_x$$

with the boundary conditions at  $x = 0$  and  $x = 1$

$$q = 0, \quad -\alpha(aq_x)_x = u - z$$

for the problem (2.1–2.2) and

$$aq_x + sq = 0,$$

$$-u_x^2 q_x + \alpha[a(aq_x)_{xx} + s(aq_x)_x] = -(a - b) u_x + a(z - u)_x + s(z - u)$$

for the problems (2.1, 2.3/4).

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