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A TRUST REGION METHOD FOR SOLVING DISTRIBUTED PARAMETER IDENTIFICATION PROBLEMS *1)

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Abstract

This paper is concerned with the ill-posed problems of identifying a parameter in an elliptic equation which appears in many applications in science and industry. Its solution is obtained by applying trust region method to a nonlinear least squares error problem. Trust region method has long been a popular method for well-posed problems. This paper indicates that it is also suitable for ill-posed problems. Numerical experiment is given to compare the trust region method with the Tikhonov regularization method. It seems that the trust region method is more promising.

Key words: Parameter identification, Ill-posed problems, Trust region.

1. Introduction

Parameter identification problems play an important role in many applications in science and industry (see [1, 3]). By parameter identification, we refers that the estimation of coefficients in a differential equation from observations of the solution to that equation. We call the coefficients the system parameters, and the solution and its derivatives the state variables. The forward problem is to compute the state variables given the system parameters and appropriate boundary conditions, which is a well-posed problems. However in parameter identification, the problems is typically ill-posed (see [5]).

For example, we consider the problem of identifying a distributed parameter $q = q(x)$ in the one-dimensional steady-state diffusion equation in the form

$$-\nabla(q\nabla u) = g, \ \text{ in } \ (0,1) \tag{1}$$

with Dirichlet boundary conditions

$$u(0) = u_0, \ u(1) = u_1.$$

This is used to model for example, the steady-state temperature distribution within a thin metal rod (see [12]). Another example is the inverse groundwater filtration problem of reconstructing the diffusivity q of a sediment from measurements of the piezometric head u in the steady state case (see [1] for further applications). We take the former case as our example. In this kind of setting, the state variable is the temperature distribution $u(x), \ x \in (0,1)$, the system parameters are diffusion coefficient $q(x)$ and the heat source term $g(x)$. The inverse problems stated here is determining parameter $q(x)$ by giving $g(x)$ and $u(x)$ for $x \in [0,1]$.

For sake of simplifying the notations, we outline the problem in the abstract operator form

$$F(q)u = g, \tag{2}$$

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where $F(q)$ represents a parameter-dependent differential operator from the parameter space Q to the state space U, $q \in Q$ represents the distributed parameter to be estimated, and $u \in U$ represents the corresponding state variable. In case of the above example, q represents the diffusion coefficient, and

$$F(q) = -\nabla(q\nabla(\cdot)).$$

Since u is the observation data, therefore, it may contain noise. Assume that the observed data can be expressed as

$$u_e = u + e \tag{3}$$

with Gaussian noise e.

Because of the ill-posedness of the problem (1), some kind of regularization technique has to be applied (see [5, 13, 24]). Perhaps Tikhonov regularization method (see [9, 20]) is the most well-known method for dealing with such kind of problems.

Given the regularization parameter $\alpha > 0$, choose $q^\alpha \in Q$ to solve the unconstrained minimization problem

$$\min_{q \in Q} M^\alpha[q] := \|F(q)u_e - g\|^2 + \alpha\|q\|^2, \tag{4}$$

where $\alpha > 0$ is called the regularization parameter and $\|q\|^2$ serves as the stabilizer.

Assume the forward problem solving for u is well-posed, then we can denote the solution by

$$f(q) := u = F^{-1}(q)g. \tag{5}$$

Clearly we want to minimize the following constrained functional

$$J_{q \in Q}(q) = \frac{1}{2}\|u - u_e\|^2, \tag{6}$$

$$s.\ t.\ F(q)u = g. \tag{7}$$

By (5), problem (6)-(7) is equivalent to the unconstrained regularized least squares minimization problem

$$\min J_{q \in Q}(q) = \frac{1}{2}\|f(q) - u_e\|^2. \tag{8}$$

Certainly we can use the Tikhonov regularization to (5), for which, we have the following minimization problem:

$$\min J_{q \in Q}(q) = \frac{1}{2}\|f(q) - u_e\|^2 + \alpha\theta(q), \tag{9}$$

where $\theta(q)$ is a regularized functional whose duty is to impose stability, $\alpha > 0$ is a regularization parameter.

This paper will deal with the problem in a different way: i.e., we use some kind of approximation to the original problem (8), then the trust region technique is used.

2. Finite Dimensional Approximation: Trust Region Method

First we introduce the trust region method in a general way. Trust region methods are a group of methods for ensuring global convergence while retaining fast local convergence in optimization algorithms. For example, we consider the minimization problem

$$\min_{x \in \mathcal{R}^n} f(x). \tag{10}$$

In trust region methods, we first choose a trial step length Δ, and then use the quadratic model to select the best step of (at most) this length for the quadratic model by solving

$$\min \psi(x_c + \xi) = f(x_c) + (g(x_c), \xi) + \frac{1}{2}(H_c\xi, \xi), \tag{11}$$

$$s.\ t.\ \|\xi\| \leq \Delta_c. \tag{12}$$

The trial step length Δ_c is considered an estimate of how far we trust the quadratic model, hence it is called a trust radius and the resultant method is called a trust region method.

In this section, we will consider the approximation minimization problem (8) by utilizing the trust region technique mentioned above.

As a rule, the numerical solution of the fundamental problem would be impossible without the use of computers. In general, the traditional way of implementation is to perform a finite-dimensional approximation of the problem under considerations.

Let P_n denote a projection of Q onto an n-dimensional subspace Q_n, i.e., $P_n : Q \longrightarrow Q_n$ and $\bar{P}_n : Q_n \longrightarrow Q$, which possess a number of remarkable properties:

(1) the operators P_n and $\bar{P}_n$ are continuous for all n;

(2) $P_n\bar{P}_n = I_n$, where I_n is the identity operator on the space X_n;

(3) $\bar{P}_nP_nq \in D(F)$ for any $q \in D(F)$ and all positive integers n.

Similarly, let R_m denote a projection of U onto an m-dimensional subspace U_m, i.e., $R_m : U \longrightarrow U_m$ and $\bar{R}_m : U_m \longrightarrow U$. Now we can define F_{mn} the finite approximation to the nonlinear operator F:

$$F_{mn}(q)u := R_mF(P_nq)u. \tag{13}$$

Now in finite dimensional case, the minimization problem is in the form

$$\min J_{q\in Q_n}(q) = \frac{1}{2}\|u - u_e\|^2, \tag{14}$$

$$s.\ t.\ F_{mn}(q)u = g. \tag{15}$$

Furthermore, if we denote $f_{mn}(q) = F_{mn}^{-1}(q)g$, (14)-(15) can be transformed into the following unconstrained minimization problem

$$\min J_{q\in Q_n}(q) = \frac{1}{2}\|f_{mn}(q) - u_e\|^2. \tag{16}$$

Since F is differentiable, each F_{mn} is differentiable. Let us denote $J_{q\in Q_n}(q)$ by J_n or $J_n(q)$, the gradient of the functional $J_{q\in Q_n}(q)$ by $grad(J_n)$, the approximate Hessian of the functional $J_{q\in Q_n}(q)$ by $Hess(J_n)$. At each iteration, a trial step is calculated by solving the subproblem

$$\min_{s\in Q_n} \phi_k(s) := grad(J_n)_k^T s + \frac{1}{2}(Hess(J_n)_k s, s), \tag{17}$$

$$s.\ t.\ I(s) \leq \Delta_k, \tag{18}$$

in finite spaces Q_n and U_m. For simplicity, we assume that $m \equiv n$. In the above expression, $I(s)$ denotes some kind of modular. For example, we can take $I(s)$ as $\frac{1}{2}\|s\|_{l^2}^2$. Here, for our purpose, we take $I(s)$ as $\frac{1}{2}\|Ls\|^2$, where L denotes some kind of discrete differential operator, which is bounded, self-adjoint positive or semi-positive definite. In (17)-(18), $grad(J_n)_k$ is the gradient at the current approximate solution, $Hess(J_n)_k$ is an $n \times n$ symmetric matrix which approximates the Hessian of $J_{q\in Q_n}(q)$ and $\Delta_k > 0$ is a trust region radius. Let s_k be a solution of (17)-(18). The predicted reduction is defined by the reduction in the approximate model, i.e.,

$$Pred_k = \phi_k(0) - \phi_k(s_k) = -\phi_k(s_k). \tag{19}$$

Unless the current point q_k is a stationary point and $Hess(J_n)_k$ is positive semi-definite, the predicted reduction is always positive. The actual reduction is the reduction in the objective function

$$Ared_k = J_{q\in Q_n}(q_k) - J_{q\in Q_n}(q_k + s_k). \tag{20}$$

And we define the ratio between the actual and the predicted reduction by

$$r_k = \frac{Ared_k}{Pred_k} \tag{21}$$

which is used to decide whether the trial step is acceptable and to adjust the new trust region radius.

With the above analysis, we generate the trust region algorithm for solving parameter identification problem as follows.

Algorithm 2.1. *(Trust region algorithm for parameter identification problem)*

STEP 1 *Given the initial guess value* $q_1 \in \mathcal{R}^n$, $\Delta_1 > 0$, $0 < \tau_3 < \tau_4 < 1 < \tau_1$, $0 \le \tau_0 \le \tau_2 < 1$, $\tau_2 > 0$, $k := 1$;

STEP 2 *If* **the stopping rule is satisfied** *then STOP; Else, solve (17)-(18) giving* s_k;

STEP 3 *Compute* r_k;

$$q_{k+1} = \begin{cases} q_k & if \quad r_k \le \tau_0, \\ q_k + s_k & otherwise; \end{cases} \tag{22}$$

Choose Δ_{k+1} *that satisfies*

$$\Delta_{k+1} \in \begin{cases} [\tau_3\|s_k\|, \tau_4\Delta_k] & if \quad r_k < \tau_2, \\ [\Delta_k, \tau_1\Delta_k] & otherwise; \end{cases} \tag{23}$$

STEP 4 *Evaluate* $grad(J_n)_k$ *and* $Hess(J_n)_k$; *k:=k+1; GOTO STEP 2.*

The constant τ_i $(i = 0, \cdots, 4)$ can be chosen by users. Typical values are $\tau_0 = 0$, $\tau_1 = 2$, $\tau_2 = \tau_3 = 0.25$, $\tau_4 = 0.5$. For other choices of those constants, please see [6], [7], [14], [17], etc.. The parameter τ_0 is usually zero (see [6], [18]) or a small positive constant (see [4] and [19]). The advantage of using zero τ_0 is that a trial step is accepted whenever the objective function is reduced. Hence it would not throw away a "good point", which is a desirable property especially when the function evaluations are very expensive (see [21]).

In STEP 2, the stopping rule is based on the so-called discrepancy principle, which will be stated in the next section.

There are several ways to evaluate the gradient of the leat squares cost functional, say, finite differences method, adjoint or costate methods (see [1], [3], [23]). For finite differences method, for example, assuming a discretization of the parameter of the form

$$q = \sum_{i=1}^{n} c_i\psi_i,$$

can be obtained, then the gradients can be approximated by

$$(grad(J_n(q)))_i \approx \frac{J_n(q + h_i\psi_i) - J_n(q)}{h_i}, \ i = 1, 2, \cdots, n, \tag{24}$$

where h_i is a relatively small scalar compared to the i^{th} component of the discretized parameter q. For distributed parameter identification, finite difference gradient computations are

expensive. From equations (14)-(15) we know each gradient evaluation requires n evaluations of $f_{mn}(q) = F_{mn}^{-1}(q)g$, and each computation of $F_{mn}^{-1}(q)$ entails the approximate solution of a differential equation. When n is large, gradient approximations based directly on (24) are extremely expensive, requiring $n+1$ evaluations of the functional $J_n(q)$, and hence $n+1$ solutions of the equation (2).

Adjoint or costate methods for parameter identification were introduced by Chavant and Lemonier (see [3]). These kinds of methods can remarkably reduce the cost of gradient evaluation. Consider the least squares problem:

$$J_n(q) = \frac{1}{2}\|f_{mn}(q) - u_e\|^2. \tag{25}$$

Letting $res(q) = f_{mn}(q) - u_e$ denote the residual and using the fact that $\frac{d}{dh}F_{mn}(q+he_i)|_{h=0} = \frac{dF_{mn}}{dq}e_i$, we obtain a representation for the components of the gradient of $J_n(q)$. For $i = 1, 2, \cdots, n$,

$$\begin{aligned}
(grad(J_n(q)))_i &:= \frac{d}{dh}J_n(q+he_i)|_{h=0} \\
&= (\frac{d}{dh}f_{mn}(q+he_i)|_{h=0}, res(q)) \\
&= -(F^{-1}(q)\frac{dF_{mn}}{dq}e_i F_{mn}^{-1}(q)g, res(q)) \\
&= (\frac{dF_{mn}}{dq}e_i u, v),
\end{aligned}$$

where u solves the state equation (15) and v solves the adjoint or costate equation

$$F_{mn}^{*}(q)v = -res(q).$$

In the above expression, $F_{mn}^{\star}$ stands for the adjoint of the operator F_{mn}.

Compared with the finite difference computation (24), the costate gradient computation requires only one inversion of the operator $F_{mn}(q)$, together with one inversion of its adjoint.

Now we turn to Hessian computations. We use Gauss-Newton method to approximate the exact Hessian of $J_{q\in Q_n}(q)$. For ease of notation, we simply denote H the exact Hessian of $J_{q\in Q_n}(q)$. In context of the least squares functional (25), its Hessian can be expressed as

$$H = Hess(J_n(q)) + \frac{d^2 f_{mn}}{dq^2}res(q), \tag{26}$$

where

$$Hess(J_n(q)) = (\frac{df_{mn}}{dq})^{\star}(\frac{df_{mn}}{dq}).$$

$Hess(J_n(q))$ is the so-called Gauss-Newton approximation to the Hessian. This evaluation has some computational advantages. First, it can sometimes be much easier to compute than the full Hessian, since it does not involve the second derivative term $\frac{d^2 f_{mn}}{dq^2}$, which has a tensor representation. Moreover, if the first derivative $\frac{df_{mn}}{dq}$ has full rank, we conclude that Gauss-Newton step is already a descent step. We can solve the original problem simply by Gauss-Newton method. But if $Hess(J_n(q))$ is singular or not singular but with small eigenvalues, we still need trust region to constrain the step. From Theorem 2.4 in the following context, we can conclude that the scaled trust region step is a strict decent direction no matter the first derivative $\frac{df_{mn}}{dq}$ has full rank or not since we can adjust the Lagrangian parameter α, such that the trust region step is a decent direction.

Take $Q_n = U_m = \mathcal{R}^n$, then for subproblem (17)-(18), we have the following lemmas. The proof of these lemmas are quite similar to [15, 19], we refer to these articles for details.

Lemma 2.2. *A vector $s^* \in \mathcal{R}^n$ is a solution of the problem*

$$\min_{s\in\mathcal{R}_n} \phi(s) := grad(J_n)^T s + \frac{1}{2}(Hess(J_n)s, s), \tag{27}$$

$$s.\ t.\ I(s) \le \Delta, \tag{28}$$

where $I(s) = \frac{1}{2}\|Ls\|^2$, L is a discrete matrix form of a bounded self-adjoint positive semi-definite linear operator, $grad(J_n) \in \mathcal{R}^n$, $Hess(J_n) \in \mathcal{R}^{n\times n}$ is a symmetric matrix, and $\Delta > 0$, if and only if there exists $\alpha^* \ge 0$ such that

$$(Hess(J_n) + \alpha^* L^* L)s^* = -grad(J_n) \tag{29}$$

and that $Hess(J_n) + \alpha^* L^* L$ is positive semi-definite, $I(s^*) \le \Delta$ and

$$\alpha^*(\Delta - I(s^*)) = 0. \tag{30}$$

Proof. By replacing the identity matrix I in [15, 19] with L^*L, the result is clear.

Lemma 2.2 establishes necessary conditions concerning the pair $\alpha^*,\ s^*$ when s^* solves (27)-(28). Our next result establishes sufficient conditions that will ensure s is a solution to (27)-(28).

Lemma 2.3. *Let $\alpha^* \in \mathcal{R},\ s^* \in \mathcal{R}^n$ satisfy*

$$(Hess(J_n) + \alpha^* L^* L)s^* = -grad(J_n) \tag{31}$$

with $Hess(J_n) + \alpha^* L^* L$ is positive semi-definite. Then we have the following results:

(1) If $\alpha^* = 0$ and $I(s^*) \le \Delta$ then s^* solves (27)-(28);

(2) If $I(s^*) = \Delta$ then s^* solves

$$\phi(s^*) = \min\{\phi(s) : I(s) = \Delta\};$$

(3) If $\alpha^* \ge 0$ and $I(s^*) = \Delta$ then s^* solves (27)-(28). Furthermore, if $Hess(J_n) + \alpha^* L^* L$ is positive definite then s^* is unique in each of cases (1), (2) and (3).

Proof. By replacing the identity matrix I in [15, 19] with L^*L, the result is clear.

From lemmas 2.2 and 2.3, we know that if $Hess(J_n) + \alpha^* L^* L$ is positive definite, s^* is uniquely defined by

$$s^* = -(Hess(J_n) + \alpha^* L^* L)^{-1} grad(J_n). \tag{32}$$

To emphasize the fact that s is dependent on the parameter α, we write

$$s_\alpha = -(Hess(J_n) + \alpha L^* L)^{-1} grad(J_n), \tag{33}$$

which has the following property:

Theorem 2.4. *Assume that L is bounded self-adjoint and positive definite, $Hess(J_n) + \alpha L^* L$ is positive definite. Then for $L = I$ (the identity operator), the norm of the search direction s_α is strictly decreasing as α increases from zero; For $L \ne I$, the norm of the scaled search direction $D^{\frac{1}{2}} s_\alpha$ is strictly decreasing as α increases from zero, where $D = L^* L$.*

Proof. First, we prove the result for $L = I$. It is easy to show

$$\frac{d}{d\alpha}\|s_\alpha\| = \frac{(s_\alpha, \frac{ds_\alpha}{d\alpha})}{\|s_\alpha\|}.$$

Differentiating the equation (33) with α for $L = I$, we have

$$(Hess(J_n) + \alpha I)\frac{ds_\alpha}{d\alpha} = -s_\alpha.$$

Hence

$$\begin{aligned}\frac{d}{d\alpha}s_\alpha &= -(Hess(J_n)+\alpha I)^{-1}s_\alpha \\ &= (Hess(J_n)+\alpha I)^{-2}grad(J_n)\end{aligned}$$

and

$$\frac{d}{d\alpha}\|s_\alpha\| = -\frac{grad(J_n)^T(Hess(J_n)+\alpha L^*L)^{-3}grad(J_n)}{\|s_\alpha\|}.$$

Since $Hess(J_n)+\alpha I$ is positive definite according to the assumption, the above relation implies that $\|s_\alpha\|$ is strictly decreasing as α increase from zero. The first assertion follows.

Next we prove the result for $L \neq I$. Noticing that $(Hess(J_n)+\alpha L^*L)^{-1}$ can be rewritten as

$$(Hess(J_n)+\alpha D)^{-1} = D^{-\frac{1}{2}}(D^{-\frac{1}{2}}Hess(J_n)D^{-\frac{1}{2}}+\alpha I)^{-1}D^{-\frac{1}{2}},$$

and if we denote $D^{-\frac{1}{2}}grad(J_n) = g_n$, then the search direction s_α can be written as

$$s_\alpha = D^{-\frac{1}{2}}(D^{-\frac{1}{2}}Hess(J_n)D^{-\frac{1}{2}}+\alpha I)^{-1}g_n.$$

Hence

$$D^{\frac{1}{2}}s_\alpha = (D^{-\frac{1}{2}}Hess(J_n)D^{-\frac{1}{2}}+\alpha I)^{-1}g_n.$$

Note that $D^{-\frac{1}{2}}Hess(J_n)D^{-\frac{1}{2}}+\alpha I$ is positive definite, the result follows for $L \neq I$ by using the same technique for the proof of $L = I$.

Theorem 2.4 is important while implementing trust region algorithm. No matter how large α is, the norms $\|s_\alpha\|$ for $L = I$ or $\|D^{\frac{1}{2}}s_\alpha\|$ for $L \neq I$ are strictly decreasing as α increases from zero. Hence, the search direction can not go everywhere.

The following theorem shows that the objective functional is monotonically decreasing.

Theorem 2.5. *Assume that L and $Hess(J_n(q_k))+\alpha L^*L$ are positive definite, q_k is the current iteration point such that $grad(J_n(q_k)) \neq 0$. Then for s a solution of (27)-(28) and Δ_k sufficiently small, we have $J_n(q_k+s) < J_n(q_k)$.*

Proof. The proof of the result is relied on the Taylor's second-order expansion. Since $J_n(q)$ is twice continuously differentiable, it follows that

$$J_n(q_k+s) = J_n(q_k) + grad(J_n(q_k))^T s + O(\|s\|^2).$$

Hence it suffices to show that when Δ_k is sufficiently small, there exists a constant $C > 0$ for which

$$grad(J_n(q_k))^T s \leq -C\|s\|. \tag{34}$$

Note that the solution s can be expressed as

$$s = -(Hess(J_n(q_k))+\alpha L^*L)^{-1}grad(J_n),$$

and by Theorem 2.4, $\|s\|$ is bounded, thus the result is clear.

From Theorem 2.5 we know that the trust region algorithm gives decrease in the objective functional outside the region of convergence (i.e., we can not trust the "trust region") and the trust region constraint $\|s\| \leq \Delta$ is active. Once the iterates are inside the region of convergence, we take the Gauss-Newton step and the trust region constraint $\|s\| \leq \Delta$ becomes inactive.

Theorem 2.5 is also important for using discrepancy principle as the stopping rule in Algorithm 2.1, see some explanation in next section.

3. Choosing Regularization Parameter and the Stopping Criterion

In inverse and ill-posed problems, regularization parameter (see equations (4) and (9)) plays an important role in quantifying the tradeoff between error amplification due to instability and truncation due to regularization. It has been developed a lot of methods for determining the regularization parameter α, we refer to [2, 5, 11, 8, 10, 16] etc. for details. Here, we will choose the regularization parameter in a different way. According to Algorithm 2.1, the trust region constraint is inactive if the current iterate is inside the trust region. In such case we accept the iterate without solving the trust region subproblem. Once the current iterate is outside the trust region, the trust region constraint is active, we have to solve the trust region subproblem. Hence our new way of choosing regularization parameter is based on the relation between the current iterate s_k and the trust region Δ_k. Note that solving for a solution s^* of the subproblem (27)-(28) is equivalent to solve the equations (29)-(30), hence the Lagrangian parameter α has to be determined in each iteration. We call such a Lagrangian parameter is a regularization parameter. This is because the small eigenvalues of $Hess(J_n)$ can be suppressed by the parameter.

We will assume that the state variable u is contaminated with error, i.e., instead of u, we may have a perturbed version u_e with error level δ such that

$$\|u - u_e\| \leq \delta.$$

In such case, the solution of the problem may be very sensitive to the small perturbations in the state variable u.

Now we introduce the trust region technique to determine the regularization parameter. Lemma 2.2 indicates that if s_k is a solution of (27) and (28), then there is a unique $\alpha_k \geq 0$ that satisfies (29) and (30). From equations (32) and (33) we know that the parameter $\alpha_k > 0$ and satisfies

$$\|s_{\alpha_k,k}\| = \Delta_k, \tag{35}$$

i.e.

$$\|(Hess(J_n(q_k)) + \alpha_k L^*L)^{-1} grad(J_n(q_k))\| = \Delta_k. \tag{36}$$

Thus, similar to techniques for subproblems of trust region algorithms for unconstrained optimization (see [21], [22]), we can apply Newton's method to the nonlinear equation

$$\Gamma_k(\alpha_k) := \frac{1}{\|s_{\alpha_k,k}\|} - \frac{1}{\Delta_k}. \tag{37}$$

The reason for considering (37) instead of the simpler equation

$$\|s_{\alpha_k,k}\| - \Delta_k = 0 \tag{38}$$

is that $\Gamma_k(\alpha_k)$ is close to a linear function. Thus Newton's method would give a faster convergence. In fact the first order and second order derivatives of $\Gamma_k(\alpha_k)$ can be easily computed, hence Newton's method can be used to calculate α^*, the solution of $\Gamma_k(\alpha_k) = 0$. For simplicity, we denote $A = Hess(J_n(q_k))$ and $b = grad(J_n(q_k))$. Applying Newton's method to (37), we can compute the iteration sequence $\{\alpha_k\}$ by the following formula

$$\alpha_+ = \alpha_k - \frac{\|s^2_{\alpha_k,k}\|}{b^T(A + \alpha_k L^*L)^{-2} L^*L (A + \alpha_k L^*L)^{-1} b} [1 - \frac{\|s_{\alpha_k,k}\|}{\Delta}] \tag{39}$$

with α^+ the next iterate.

The following algorithm updates α_k by Newton's method applied to (37).

Algorithm 3.1. *(Newton's method for computing α)*
Until convergence do

STEP 1 Factor $A + \alpha_k L^*L = R^T R$;

STEP 2 Solve $R^T R s_{\alpha_k,k} = -b$;

STEP 3 Solve $R^T R w = s_{\alpha_k,k}$;

STEP 4 Let $\alpha_k := \alpha_k - \frac{\|s_{\alpha_k,k}\|^2}{\|w^T L^* L s_{\alpha_k,k}\|}(1 - \frac{\|s_{\alpha_k,k}\|}{\|\Delta_k\|})$.

In this algorithm, the stopping rule is based on the errors of the regularization parameters,i.e. *If* $\|\alpha_{k+1} - \alpha_k\| \leq tol$, *we terminate the iteration for seeking optimal values of* α_k. $R^T R$ is the Cholesky factorization of matrix $A + \alpha_k L^*L$ with $R \in \mathcal{R}^{n\times n}$ upper triangular. It is necessary to safeguard α_k in order to obtain a positive definite $A + \alpha L^*L$ and guarantee convergence. This in practice can be satisfied by observing the fact that the function $\Gamma_k(\alpha_k)$ is concave and strictly increasing, hence if we choose the initial guess value $\hat{\alpha} > 0$ such that $\Gamma_k(\hat{\alpha}) < 0$ then at each iteration, Newton algorithm generates a monotonically increasing sequence converging to the solution of $\Gamma_k(\alpha_k) = 0$.

We should also point out that, Algorithm 3.1 can still be implemented even if L is semi-definite as long as $A + \alpha_k L^*L$ is positive definite. With the above analysis this in fact is feasible.

For the present version of trust region iteration the discrepancy principle is an appropriate stopping criterion for this purpose. Assume that

$$\|u_e - f(q_{true})\| \leq \delta$$

and to emphasize the dependency on δ we let $\{q_k^\delta\}$ denote the iterates if u_e instead of u is used in the iteration. According to the discrepancy principle the iteration is terminated at the first occurrence of the index $k = k_D$ such that

$$\|u_e - f(q_{k_D}^\delta)\| \leq \tau\delta \tag{40}$$

with $\tau > 1$ being another parameter.

This stopping rule for the trust region method is well-defined since according to Theorem 2.5, $\|u_e - f(q_k^\delta)\|$ is monotonically decreasing in k.

4. Numerical Test

We give a numerical example to test the efficiency of the proposed trust region method. Our example is based on the steady-state diffusion equation given in section 1.

The interval is chosen to be $[0, 1]$, the boundary conditions u in (1) as

$$u_0 = u_1 \equiv 0,$$

the heat source term $g(x)$ as

$$g(x) = 1$$

and the starting parameter q_1 as

$$q_1 \equiv 1.$$

We define the exact solution as $q_{true} = 1 + 0.75e^{-50(x-0.25)^2}$, then generate u according to equation (1).

To simulate the computational process by computers, all of the functions need to be in finite cases. We employ collocation method to transfer the original problem from infinite dimensional spaces to finite dimensional spaces. We apply standard piecewise linear finite element discretization with nodes $x_i = ih$, $h = 1/(n+1)$, $n = 50$. Mid-point quadrature is used to evaluate the finite element stiffness matrix, and the discrete system is formulated as follows:

$$\mathbf{F}(\mathbf{q})\mathbf{u} = \mathbf{g}.$$

Here, the black fonts mean that all of the functions are in finite cases.

To simulate the observation data, we add Gaussian noise rand$(\cdot)$ to the exact value $\mathbf{u}$ as

$$\mathbf{u_e} = \mathbf{u} + \delta \cdot \mathrm{rand}(\mathbf{u}).$$

Our problem is to estimate $\mathbf{q}$ given the observation data $\mathbf{u_e}$. We consider the approximation problem to least squares functional $\mathbf{J}(\mathbf{q}) = \|\mathbf{F^{-1}}(\mathbf{q})\mathbf{g} - \mathbf{u_e}\|^2$:

$$\phi(s) := grad(\mathbf{J})^T s + \frac{1}{2}(Hess(\mathbf{J})s, s), \tag{41}$$

$$s.\ t.\ I(s) \le \Delta, \tag{42}$$

where $I(s) = \frac{1}{2}\|\mathbf{L}s\|^2$, $\mathbf{L}$ is the discrete one-dimensional negative Laplacian with homogeneous natural boundary conditions:

$$\mathbf{L} = \frac{1}{h}\begin{bmatrix} 1 & -1 & 0 & \cdots & 0 & 0 \\ -1 & 2 & -1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \cdots & \vdots & \vdots \\ 0 & 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & \cdots & -1 & 1 \end{bmatrix}.$$

First, trust region Algorithm 2.1 is implemented to solve the above problem. The results are shown in Figure 1–Figure 4.

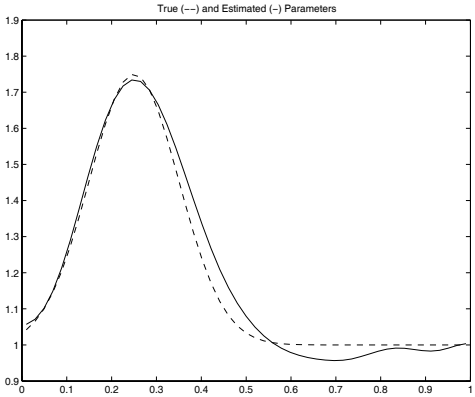

Figure 1

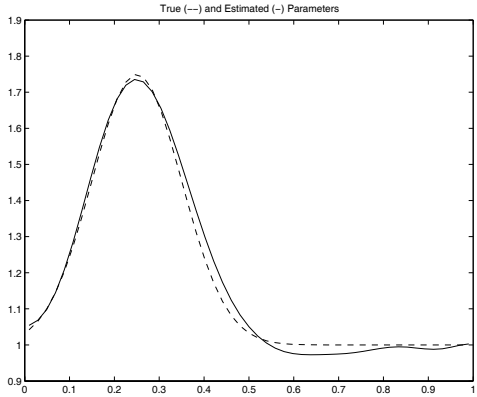

Figure 2

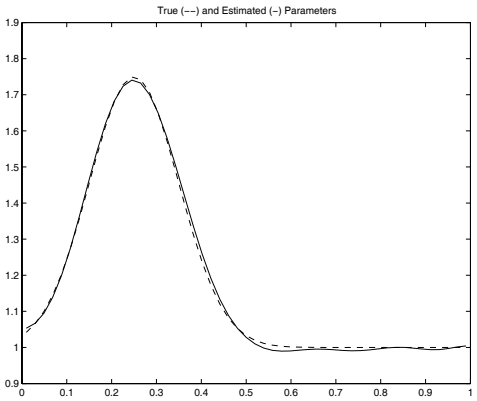

Figure 3

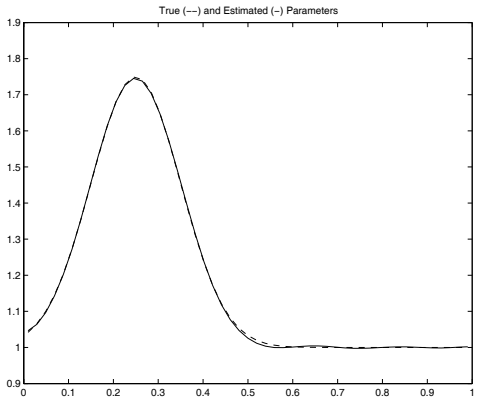

Figure 4

In all the figures, we choose the initial trust region radius as $\Delta_1 = 1.0$, the initial guess value of α as 0.1, the dominant parameter τ as 1.01. The error levels we used and the iterations are displayed in Table 1. We observe from figure 3 and figure 4 that if the error level is small, then the approximated solution can approximate the exact solution perfectly well. Note that the choice the initial guess value α is not so crucial. We have tested on other initial choices of α values, say $\alpha = 5, 10$ or 100, and got the same results. Another interesting fact in our experiment is, *though the values of the parameters α_k are increasing in each inner iteration, which are generally decreasing to zero (by recording the last values of α_k in each loop of Algorithm 3.1).*

Table 1 The error levels and the iterations

	error level (δ)	iterations
Figure 1	$\delta = 2\%$	15
Figure 2	$\delta = 1\%$	16
Figure 3	$\delta = 0.5\%$	18
Figure 4	$\delta = 0.1\%$	22

We also perform Tikhonov regularization (9) to solve the diffusion equation. The stabilizer $\theta(\mathbf{q})$ is chosen as $\frac{1}{2}\|\mathbf{Lq}\|^2$, $\mathbf{L}$ is the discrete one-dimensional Laplacian. We use quasi-Newton iteration to minimize Tikhonov functional

$$\frac{1}{2}\|\mathbf{F^{-1}(q)g} - \mathbf{u_e}\|^2 + \alpha\theta(\mathbf{q})$$

and the computational results are shown in Figure 5–Figure 8. The error levels we used and the iterations are displayed in Table 2. We use an *a-priori* estimation of the regularization parameter α. In all of the figures 5–8, we choose the regularization parameter α as 0.1, the dominant parameter τ as 2.0. Note that this choice of the regularization parameter is crucial. It can not be too large or too small. If α is too large, its solution may be far from the noise-free solution since the new problem is a poor approximation to the original problem; if α is too small, the influence of the data errors may cause instabilities. We can see this phenomena from figures 6, 9 and Figure 10. We add the same noise level $\delta = 0.01$ in these figures. In Figure 9 we choose $\alpha = 5.0$, in Figure 10 we choose $\alpha = 1.0 \times 10^{-4}$. If α is larger than 5.0 or smaller than 1.0×10^{-4}, the results will be more worse.

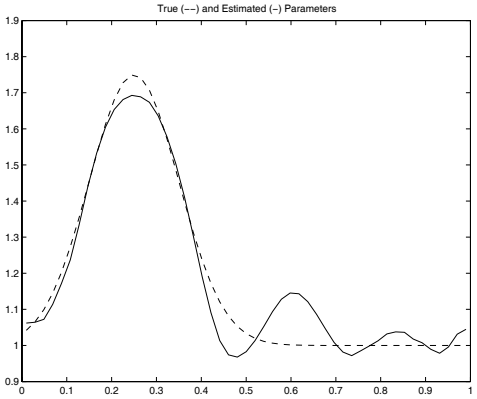

Figure 5

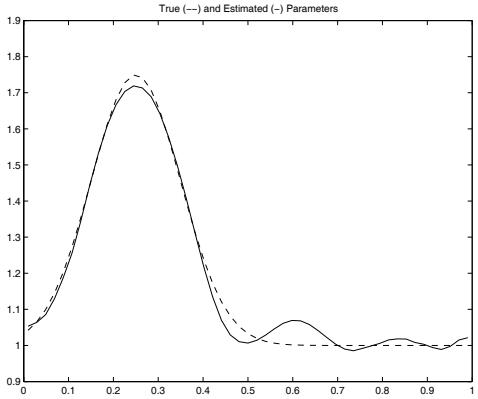

Figure 6

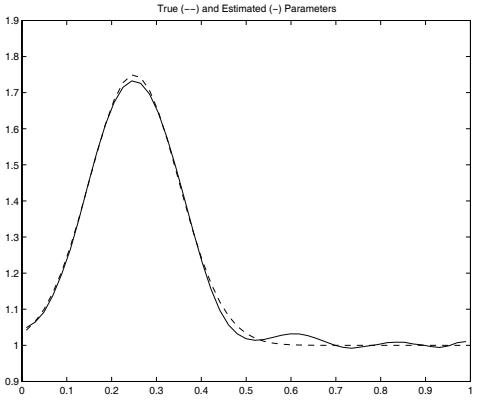

Figure 7

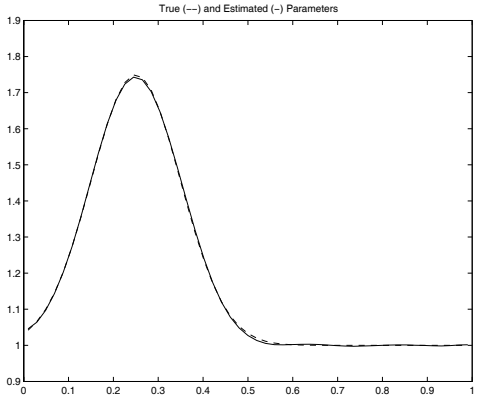

Figure 8

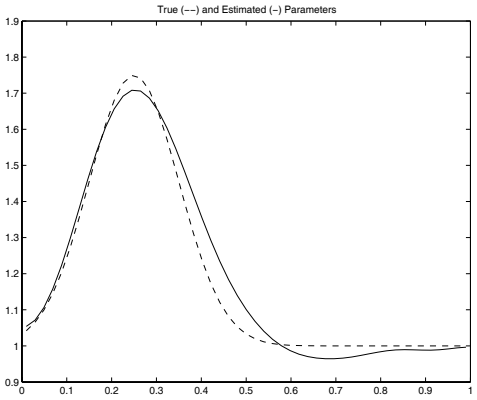

Figure 9

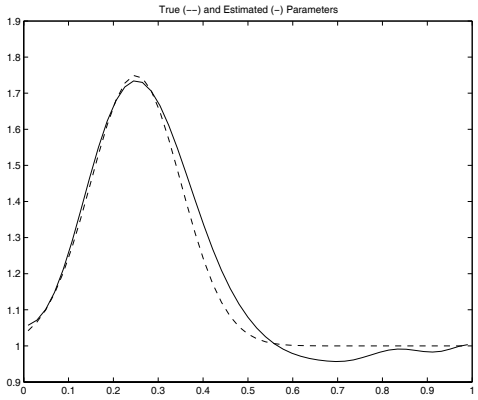

Figure 10

Table 2 The error levels and the iterations

	error level (δ)	iterations
Figure 5	$\delta = 2\%$	2
Figure 6	$\delta = 1\%$	2
Figure 7	$\delta = 0.5\%$	3
Figure 8	$\delta = 0.1\%$	3
Figure 9	$\delta = 1\%$	2
Figure 10	$\delta = 1\%$	3

From Figure 1–Figure 8, we observed that the behavior of the trust region method and the Tikhonov regularization method is very similar. They are both stable methods. We also observed from Figure 3–Figure 4 and Figure 7–Figure 8 that if the error level is small, the solution obtained by trust region method can approximate the exact solution as well as by Tikhonov regularization method.

5. Conclusion and Future work

The numerical experiment illustrates that the trust region method is stable for solving ill-posed problems, at least for distributed parameter identification problem concerned in this paper. We do not claim that the trust region algorithm is better than Tikhonov regularization, which has been developed for about 40 years starting from the basic works by Tikhonov. But at least it can give a comparative results. We may conclude that the trust region technique is suitable for regularizing ill-posed problems. But how to prove the regularity of the trust region algorithm remains an interesting topic, we will give a further research later.

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