A Numerical Method to Estimate the Optimal Regularization Parameter

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In this paper, we propose a numerical method to estimate the optimal regularization parameter based on a previous paper [12]. Using the singular value decomposition, the method estimates the optimal parameter efficiently in the course of calculation of the solution. Some numerical examples applied to Fredholm integral equations of the first kind are presented.

1. Introduction

In the present paper, on the basis of a previous paper [12], we develop an efficient numerical algorithm to estimate the optimal parameter in the regularization method for solving linear ill-posed problems including Fredholm integral equations of the first kind. Let F and G be Hilbert spaces and $\bar{T}$ be a linear compact operator acting from F to G and consider an operator equation

$$\bar{T}\bar{f}=\bar{g}, \tag{1.1}$$

where $\bar{f}\in F$ and $\bar{g}\in G$. The equation (1.1) includes as a special case Fredholm integral equations of the first kind of the form

$$\int_a^b K(s,t)\bar{f}(t)\,dt=\bar{g}(s), \quad s_{min}\leqq s\leqq s_{max} \tag{1.2}$$

where $K(s, t)$ and $\bar{g}(s)$ are known L_2 functions and $\bar{f}(t)$ is the unknown function in $L_2[a, b]$.

We suppose that the operator equation (1.1) is discretized by some method into the linear system of the form

$$\hat{T}\hat{f}=\hat{g}, \tag{1.3}$$

with $\hat{f}=(\hat{f}_1, \hat{f}_2, \ldots, \hat{f}_n)\in \mathbf{R}^n$, $\hat{g}=(\hat{g}_1, \hat{g}_2, \ldots, \hat{g}_m)\in \mathbf{R}^m$ and $\hat{T}:\mathbf{R}^n\rightarrow\mathbf{R}^m$. An example of the discretization is given in the numerical examples of Section 5. Let $(\cdot, \cdot)$ denote the inner product and $\|\cdot\|$ the Euclidean norm in the sequel. In the case of a rectangular matrix T, we define the condition number of T by $\|T^{\dagger}\|\|T\|$.

If the operator $\bar{T}$ does not have a bounded inverse, then the condition number of the matrix $\hat{T}$ increases rapidly as m and n increase. (For the equation (1.2) the speed depends on the smoothness of the kernel K(s, t).) Hence, the ordinary least squares method does not work out well for this kind of problems. One well known technique to overcome the difficulty of this ill-conditioning involves the method of regularization [8, 9, 11, 17]. The method converts (1.3) to a minimization problem which can be stated that

find $\hat{f}\in \mathbf{R}^n$ for which

$$\min_{\hat{f}\in \mathbf{R}^n}\{\|\hat{T}\hat{f}-\hat{g}\|^2+\mu\|L\hat{f}\|^2\}, \tag{1.4}$$

is attained, where L is a discretizaition of an operator of the Hilbert space F into itself which is called a stabilizer and μ is a parameter. The functional to be minimized in (1.4) is called the smoothing functional whose minimizer $\hat{f}$ is the solution of the normal equation of the form

$$(\hat{T}^t\hat{T}+\mu L^tL)\hat{f}=\hat{T}^t\hat{g}. \tag{1.5}$$

The stabilizer usually involves the norm of the solution $\bar{f}$ or derivative of $\bar{f}$ for the integral equation problem. An example of the stabilizer is given in Section 5. The parameter μ is called the regularization parameter which plays a vital role for controlling the stability of the equation (1.5).

Though this method is known to be very successful in practice, it has a critical drawback that one should choose the regularization parameter which is optimal in some sense. The selection of the parameter μ decides how well the method approximates the solution [1, 5, 8, 14, 17, 20]. In this paper, we develop an algorithm to estimate the parameter automatically and efficiently.

By numerical procedures stated in Section 3, we can transform the functional in (1.4) into that with L=I. (Then $\hat{T}$, $\hat{f}$ and $\hat{g}$ are transformed to T, f and g respectively). Then we can formulate our problem as follows:

For given g and $g_\Delta=g+\Delta g\in \mathbf{R}^m$, find $f=f(\mu;\Delta g)\in \mathbf{R}^n$ and $\mu\in[0,\infty)$ for which

$$\min_{f\in \mathbf{R}^n}\{\|Tf-g_\Delta\|^2+\mu\|f\|^2\} \tag{1.6}$$

and

$$\min_{\mu\in[0,\infty)}\|T^{\dagger}g-f(\mu;\Delta g)\|^2 \tag{1.7}$$

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are attained, where $T^\dagger$ denotes the Moore-Penrose generalized inverse [7], [14] of T and $f(\mu; \Delta g)$ in (1.7) represents the minimizer of the smoothing functional (1.6).

The main purpose of this paper is to design an efficient numerical scheme to solve the problem of (1.6) and (1.7), in other words, to estimate the optimal regularization parameter μ_0 which is defined as follows.

Definition 1.1 *We call μ_0 the optimal regularization parameter if*

$$\mu_0 \in \{\bar{\mu} \mid \min_{\mu \in [0,\infty)} \|T^\dagger g - f(\mu; \Delta g)\| = \|T^\dagger g - f(\bar{\mu}; \Delta g)\|\}.$$

Note that μ_0 is the minimizer of (1.7). First, in Section 2, we prepare several notations and present an outline of the theory developed in [12]. Next, in Section 3, we construct an effective algorithm which will be numerically implemented. Furthermore, in Section 4, we give a summary of the algorithm. Finally, in Section 5, we present results of some numerical experiments which show how the numerical scheme works well in practice.

2. Preliminaries

In this section we prepare mathematical foundations and the notations required in the sequel. We also outline our previous paper [12] on which the algorithm developed in the later section is based.

For any m by n matrix T with $m \geqq n$, there exist singular values $\{\sigma_i\}, i=1, 2, \ldots, n$, m by m unitary matrix U and n by n unitary matrix V such that

$$T = U\Sigma V^t, \tag{2.1}$$

where Σ is m by n matrix with $\Sigma = \mathrm{diag}(\sigma_1, \sigma_2, \ldots, \sigma_n)$ and V^t denotes the transpose of V [4], [6]. We assume that $\sigma_1 \geqq \sigma_2 \geqq \ldots \geqq \sigma_n \geqq 0$. Note that column vectors $\{\mathbf{u}_i\}, i=1, \ldots, m$ of U and $\{\mathbf{v}_i\}, i=1, 2, \ldots, n$ of V form orthonormal bases of $\mathbf{R}^m$ and $\mathbf{R}^n$ respectively.

Hereafter, we write $f(\mu) = f(\mu; \Delta g)$, etc. for simplicity. Using the singular values and the vectors, we can write the minimizer $f(\mu)$ of the functional in (1.6) as

$$f(\mu) = (T^tT + \mu I)^{-1}T^t(g + \Delta g) \tag{2.2}$$

$$= \sum_{i=1}^{n} \frac{\sigma_i}{\sigma_i^2 + \mu}(\tilde{g}_i + \Delta\tilde{g}_i)\mathbf{v}_i, \tag{2.3}$$

or

$$\tilde{f}_i(\mu) = \sum_{i=1}^{n} \frac{\sigma_i}{\sigma_i^2 + \mu}(\tilde{g}_i + \Delta\tilde{g}_i), \tag{2.4}$$

where $\tilde{f}(\mu) = V^t f(\mu)$, $\tilde{g} = U^t g$ and $\Delta\tilde{g} = U^t\Delta g$ with $\tilde{f}(\mu) = (\tilde{f}_1(\mu), \tilde{f}_2(\mu), \ldots, \tilde{f}_n(\mu))^t$, $\tilde{g} = (\tilde{g}_1, \tilde{g}_2, \ldots, \tilde{g}_n)^t$ and $\Delta\tilde{g} = (\Delta\tilde{g}_1, \Delta\tilde{g}_2, \ldots, \Delta\tilde{g}_n)^t$.

Similarly $T^\dagger g$ can be written as

$$T^\dagger g = \sum_{i \in \Gamma} \frac{1}{\sigma_i}\tilde{g}_i\mathbf{v}_i, \quad \text{where } \Gamma = \{i \mid \sigma_i \neq 0\} \tag{2.5}$$

or

$$(\tilde{T}^\dagger\tilde{g})_i = \begin{cases} \frac{1}{\sigma_i}\tilde{g}_i & \text{if } i \in \Gamma, \\ 0 & \text{if } i \notin \Gamma, \end{cases} \tag{2.6}$$

where $\tilde{T}^\dagger = V^t T^\dagger U$.

To estimate μ_0, we introduce first two vector valued functions $\tau(\mu) = (\tau_1(\mu), \tau_2(\mu), \ldots, \tau_n(\mu))$ and $\eta(\mu) = (\eta_1(\mu), \eta_2(\mu), \ldots, \eta_n(\mu))$ defined as follows:

Let $e(\mu; \Delta g) = T^\dagger g - f(\mu; \Delta g)$, $\tilde{e}(\mu; \Delta g) = V^t e(\mu; \Delta g) \equiv \tilde{T}^\dagger\tilde{g} - \tilde{f}(\mu, \Delta g)$, $\tau(\mu) = \tilde{e}(\mu; 0)$ and $-\eta(\mu) = \tilde{e}(\mu; \Delta g) - \tilde{e}(\mu; 0)$. Note that $e(\mu; \Delta g)$ is in (1.7) whose norm should be minimized with respect to μ. We may write $e(\mu) = e(\mu; \Delta g)$ etc for simplicity. Then it directly follows from (2.4) and (2.5) that

$$\tau_i(\mu) = \frac{\mu}{\sigma_i^2(\sigma_i^2 + \mu)}\tilde{g}_i, \quad i = 1, 2, \ldots, n \tag{2.7}$$

and

$$\eta_i(\mu) = \frac{\sigma_i}{\sigma_i^2 + \mu}\Delta\tilde{g}_i, \quad i = 1, 2, \ldots, n. \tag{2.7}$$

We call $\tau(\mu)$ theoretical error vector function and $\eta(\mu)$ computational error vector function. Namely, $\tau(\mu)$ represents the error due to the regularization without the perturbation Δg, while $\eta(\mu)$ represents the error introduced to regularized solution due to the perturbation Δg. We also have the relation $\tilde{e}(\mu) = \tau(\mu) - \eta(\mu)$ and $\|\tilde{e}(\mu)\| = \|e(\mu)\|$

As for these error vector functions, we have the following: $\|\tau(\mu)\|$ is monotone increasing with respect to $\mu > 0$ and $\|\eta(\mu)\|$ is monotone decreasing with respect to $\mu > 0$ (Lemma 2.1 of [12]). The way to estimate μ_0, developed in [12] is as follows: (Since the following idea is quite heuristic, please refer to [12] for the rigorous discussion):

(a) Since $\|\tau(\mu)\|$ and $\|\eta(\mu)\|$ are monotone increasing and decreasing respectively, there should be regions in which $\|\tau(\mu)\| > C\|\eta(\mu)\|$ holds and in which $C\|\tau(\mu)\| < \|\eta(\mu)\|$ holds for some $C > 1$. We call the former the theoretical error dominant region Ω_τ and the latter the perturbation error dominant region Ω_η. (Definition 2.3 and Theorem 2.1 of [12]).

(b) We may think that $\|e(\mu)\|$ is nearly equal to $\|\tau(\mu)\|$ in Ω_τ and $\|e(\mu)\|$ is nearly equal to $\|\eta(\mu)\|$ in Ω_η and accordingly the monotonicity of $\|\tau(\mu)\|$ and $\|\eta(\mu)\|$ inherits to $\|e(\mu)\|$ in each region. In other words, $\|e(\mu)\|$ is monotone increasing in Ω_τ, and monotone decreasing in Ω_η. This is actually true under some conditions. (Theorem 4.1 and Theorem 5.1 of [12]) Thus the optimal parameter μ_0 lies in the optimal region $\Omega_0 \equiv [0, \infty) \backslash (\Omega_\tau \cup \Omega_\eta)$.

(c) Since the optimal parameter μ_0 satisfies

$$\frac{d}{d\mu}\|\tilde{e}(\mu)\|\Big|_{\mu=\mu_0} = 0,$$

it seems natural to estimate μ_0 by minimizing some upper bound of

$$\left|\frac{d}{d\mu}\|\tilde{e}(\mu)\|\right|.$$

One of the conceivable upper bounds for it may involve $\|df(\mu)/d\mu\|$ which directly follows from the relation of $e(\mu)=\bar{T}^{\dagger}g-f(\mu)$.

(d) We introduce a function

$$\zeta:\mu \longrightarrow \left\|\frac{d}{d\xi}f(\mu)\right\|^2, \quad \xi=\log_{\beta}\mu \tag{2.8}$$

for some $\beta>1$ to estimate the optimal regularization parameter μ_0. Then for any $\mu\in[0, \infty)$, we have

$$\left|\frac{d}{d\xi}\|\tilde{e}(\mu)\|\right| \leqq \left\|\frac{d}{d\xi}\tilde{f}(\mu)\right\| \tag{2.9}$$

(Lemma 6.1 of [12]). Note that $d\|\tilde{e}(\mu)\|/d\xi \gtreqless 0$ is equivalent to $d\|\tilde{e}(\mu)\|/d\mu \gtreqless 0$. We expect that the minimizer of ζ is close to the optimal regularization parameter μ_0.

(e) Though we cannot assert that the minimizer μ_ζ of $\zeta(f;\mu)$ coincide with μ_0, under some conditions the minimizer among $\mu\in P_\sigma$, where P_σ is the set of singular values of T^tT, is in $\bar{\Omega}_0$, the extension of Ω_0 to the closest singular values of T^tT. (Definition 6.1 and Theorem 6.1 of [12])

In this paper, we develop an efficient algorithm based on the above idea and examine how the method works in actual problems.

3. Construction of Algorithm

Our original problem is given by (1.6) and (1.7). In place of (1.7), we introduce the function (2.8) to estimate the optimal regularization parameter. We write the function ζ introduced in (2.8) $\zeta(f;\mu)$ hereafter. Our new problem becomes as follows:

For given g and $g_\Delta=g+\Delta g\in \mathbf{R}^m$, find $f=f(\mu;\Delta g)\in\mathbf{R}^n$ and $\mu\in[0, \infty)$ for which (1.6) and

$$\min_{\mu\in[0,\infty)} \zeta(f;\mu) \tag{3.1}$$

are attained. The minimization problem (1.6) is equivalent to solving the normal equation of the form

$$(T^tT+\mu I)f=T^tg_\Delta. \tag{3.2}$$

The formulation of the regularization may be made by more general setting with a stabilizer L of the form of (1.5). The normal equation (3.2) is called standard form and the equation in the form of (1.5) can be transformed to the standard form. This can be done by using an algorithm given in Voevodin [19] in the case where L is nonsingular and in Elden [2] in the case where L is singular. For the completeness of the algorithm, we here briefly sketch the Voevodin's procedure and see how (1.5) can be transformed to (3.2). First we factor L^tL in the normal equation by the Cholesky decomposition as

$$L^tL=R^tR \tag{3.3}$$

where R is upper triangular matrix. Then normal equation (1.5) becomes

$$(\hat{T}^t\hat{T}+\mu R^tR)\hat{f}=\hat{T}^t\hat{g}. \tag{3.4}$$

Operating $(R^t)^{-1}$ from left and setting $T=\hat{T}R^{-1}$, $f=R\hat{f}$ and $g_\Delta=\hat{g}$, we have the standard form of (3.2).

This enables us to reduce our problem to the combination of (3.2) and (3.1). Our main concern in developing an efficient algorithm involves the following points:

i) Since we should seek the minimizer $f(\mu)$ of (1.6) for various values of μ, arithmetic operation count required to obtain $f(\mu)$ for each regularization parameter μ is of great concern.

ii) Since the function $\zeta(f;\mu)$ is neither convex nor concave, at what points of μ we should evaluate the values of ζ to find the minimizer.

In our approach, usage of the singular value decomposition is essential from above two aspects. As for (i), if we solve (3.2) by conventional method like Gaussian elimination, then $O(n^3)$ arithmetic operations are required to obtain f for each μ. We should vary μ for a wide range to seek the minimizer of (3.1). Moreover we note that, as is well known, the condition number of a matrix T is squared when one make T^tT explicitly. We should avoid this situation.

By performing singular value decomposition on T in the normal equation of the standard form (3.2), we have $T=U\Sigma V^t$ where $U=[\mathbf{u}_1, \mathbf{u}_2, \ldots \mathbf{u}_m]$, $\Sigma=\mathrm{diag}(\sigma_1, \sigma_2, \ldots, \sigma_n)$ and $V=[\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n]$ with $\mathbf{u}_i$'s and $\mathbf{v}_j$'s are singular vectors and σ_i's are singular values. Using the matrices U, V and Σ, we can transform the normal equation of the standard form (3.2) into

$$(\Sigma^t\Sigma+\mu I)\tilde{f}=\Sigma^t\tilde{g}_\Delta. \tag{3.5}$$

where $\tilde{f}=V^tf$ and $\tilde{g}_\Delta=U^tg_\Delta$. Corresponding to (3.5), we transform the function $\zeta(f;\mu)$ to $\zeta(\tilde{f};\mu)$. Since the matrix V is orthogonal, we have $\|\tilde{f}\|=\|V^tf\|=\|f\|$, and accordingly the minimizer in (3.1) is invariant under the transformation V. Thus we can replace $\zeta(f;\mu)$ by $\zeta(\tilde{f},\mu)$. Note that once the normal equation (3.2) is transformed to (3.5), the arithmetic operation count required to obtain $\tilde{f}(\mu)$ and $\zeta(\tilde{f};\mu)$for each μ is only O(n). Moreover, since $\tilde{f}(\mu)$ can be calculated by the formula (2.4), we do not have to construct T^tT explicitly and can avoid extra numerical instability.

As to (ii), since Theorem 6.1 of [12] asserts that under some conditions the minimizer of $\zeta(\mu)$ among $\mu\in P_\sigma$ lies in the optimal region $\bar{\Omega}_0$, we may seek the minimizer only in the set P_σ which is the set of singular values of T^tT. Since the set P_σ consists of at most n elements and the arithmetic operation count required to calculate $\zeta(\tilde{f};\mu)$ for each μ is O(n), the total operation count for $\zeta(\tilde{f};\mu)$ to find its minimizer over P_σ amounts to $O(n^2)$.

Taking all these in consideration, our final algorithm is the combination of (3.5) and

$$\min_{\mu\in P_\sigma} \zeta(\tilde{f};\mu) \tag{3.6}$$

instead of (1.6) and (3.1). After finding the pair (μ, $\tilde{f}(\mu)$), we transform $\tilde{f}$ to f by $f = V\tilde{f}$ which requires $O(n^2)$ arithmetic operations. We also note that the solution $\tilde{f}(\mu)$ of (3.5) can be computed by the formula (2.4).

All in all, the major part of calculation resides in the transformation of (3.2) to (3.5) by the singular value decomposition which costs $O(n^3)$ operations [2].

4. Summary of the Numerical Algorithm

Suppose that the problem is given in the standard form of (1.6) or (3.2), otherwise convert it to the standard form by Voevodin's or Elden's procedure [2, 18]. Note that we require only g_Δ for our algorithm and exact g is not necessarily known in practice.

Step 1. By singular value decomposition $T = U\Sigma V^t$, transform it to (3.5).

Step 2. For $i = 1, 2, \ldots, n$, set $\mu = \sigma_i^2$ and compute corresponding $\tilde{f}$ (not f) by the formula (2.4). At the same time compute the corresponding value of $\zeta(\tilde{f}; \mu)$.

Step 3. Find μ in P_σ which minimizes $\zeta(\tilde{f}; \mu)$ and using the μ obtain the final regularaized solution f by $f(\mu) = V\tilde{f}(\mu)$.

Remark: The strategy to estimate the optimal parameter μ_0 may be modified in the final stage. For example, one can seek the minimal point of $\zeta(f; \mu)$ at the neighborhood of the minimizer $\mu \in P_\sigma$. This modification seems to be reasonable since we have the inequality (2.8) and the estimation might be more reliable. We employ this modification in the numerical examples.

5. Numerical Examples

5.1 Discretization

For the example of the algorithm in practice, we test Fredholm integral equations of the first kind with smooth kernel. Theoretical foundation of the algorithm has been given in the previous paper [12] under some assumptions on σ_i, $\tilde{g}_i$, $\Delta\tilde{g}_i$ etc. Although we cannot verify the assumptions in practical problems, results of the numerical experiments show that the algorithm gives good estimations for wide range of Δg.

We employ 'cubic B-spline' [16] as the basis for the solution $\bar{f}(t)$ since (i) spline's local supportedness results in quick computation of the integrals for the discretization, (ii) spline's local supportedness also leads to a band structured matrix for the stabilizer L. The discretization proceeds as follows: Given an original integral equation of the form

$$\int_a^b K(s, t)\bar{f}(t)\,dt = \bar{g}(s), \quad s_{min} \leqq s \leqq s_{max} \tag{5.1}$$

We approximate the solution $\bar{f}(t)$ by the linear combination of spline's functions $\phi_i(t)$, $i = 1, \ldots, n$,

$$\bar{f}(t) = \sum_{i=1}^{n} \hat{f}_i\phi_i(t).$$

For the first variable s we employ m equidistant points. Then we have the normal equation in general form

$$(\hat{T}^t\hat{T} + \mu L^tL)\hat{f} = \hat{T}^t\hat{g}. \tag{5.2}$$

where

$$\hat{T} = (\hat{\tau}_{ij}), \quad \hat{\tau}_{ij} = \int_a^b K(s_i, t)\phi_j(t)\,dt,$$
$$L^tL = (\rho_{kj}), \ \rho_{kj} = \int_b^a \phi_k(t)\phi_j(t)\,dt$$

with $i = 1, 2, \ldots, m$, $k, j = 1, 2, \ldots, n$, and

$$\hat{g} = \{\bar{g}(s_1), \bar{g}(s_2), \ldots, \bar{g}(s_m)\}^t,$$
$$\hat{f} = \{\hat{f}_1, \hat{f}_2, \ldots, \hat{f}_n\}^t.$$

Making use of Voevodine's procedure, we transform the normal equation (5.2) to the standard form. In the following examples, the integration is done by 3-point Gaussian quadrature.

To examine the effectiveness of the algorithm, we contaminate the given $\hat{g}$ by some perturbation $\Delta\hat{g}$, where $\Delta\hat{g}$ is independent and normally distributed with mean 0 and standard deviation δ.

5.2 Explanation of notations and notions

(1) The true solution $\bar{f}(t)$: The solution of given Fredholm integral equations of the first kind.

(2) n: Number of basis functions (Cubic B-spline). Number of subdivision of the domain of the solution+3. For instance, $n = 19$ means the number of subdivision is 16.

(3) m: The number of the collocation points.

(4) s_i: The location of the m equidistant points where $\bar{g}(s)$ is given. $i = 1, 2, \ldots, m$.

(5) $\|T\|$: The spectral norm of the discretized matrix T in the standard form, or the largest singular value of T.

(6) Numerical Rank of T: The number of singular values larger than the round off level of computation.

(7) Noise Level: The standard deviation δ of the perturbation $\Delta\hat{g}$ which is a vector of normally distributed random numbers with mean 0. In the case where $\Delta\hat{g}$ is the round off error, we write noise Level = round off.

(8) $\|e(\mu_0)\|$: Max norm error of the optimal solution which is computed using the optimal parameter μ_0, namely

$$\|e(\mu_0)\| = \|\bar{f}(t) - \sum_{i=1}^{n} \hat{f}_i(\mu_0)\phi_i(t)\|,$$

(9) $\|e(\mu_\zeta)\|$: Max norm error of the solution which is computed using the estimated parameter μ_ζ which is the minimizer of $\zeta(f; \mu)$, namely

$$\|e(\mu_\zeta)\| = \|\bar{f}(t) - \sum_{i=1}^{n} \hat{f}_i(\mu_\zeta)\phi_i(t)\|,$$

(10) Ratio of precision: This is a measure of performance of the estimation of the parameter defined by Ratio of Precision $\equiv \log_e(\|e(\mu_\zeta)\|)/\log_e\|e(\mu_0)\|$. This in-

dicates how accurately μ_0 is estimated. If the ratio=1, the estimation attains the full accuracy.

5.3 Keys to figures and tables

μ: The regularization parameter.

x-axis: $-\log_{10}$(regularization parameter μ).

y-axis: $\log_{10}$(maximum error of the regularized solution $\|e(\mu)\|$.

$\|e(\mu)\|$: Maximum error of the regularized solution defined by

$$\|e(\mu)\| = \max_{t \in [a,b]} |\bar{f}(t) - \sum_{i=1}^{n} \hat{f}_i(\mu)\phi_i(t)|.$$

$\zeta(\mu)$: The function to estimate the optimal regularization parameter given by (3.1).

In figures Fig. 1-6, the vertical lines show the location of the squares of the singular values of T in logarithmic scale with basis 10. In the following examples, the numerical rank of T is smaller than n. This means the smallest singular value of T is smaller than the round off error level and the matrix T is extremely ill-conditioned. The tables show only critical part of the neighborhood of the minima of $\zeta(\mu)$ and $\|e(\mu)\|$ for brevity. The global behaviors of them can be observed by figures. All the numerical experiments are done by double presicion of Apollo Domain DN-3000 which has accuracy of

Table 1 Example 1 Noise Level=round off

μ	$\zeta(\mu)$	$\|e(\mu)\|$
0.100E−09	0.131E−05	0.8303E−05
0.316E−10	0.142E−05	0.5832E−05
0.100E−10	0.874E−08	0.2882E−05
0.316E−11	0.366E−06	0.1033E−05
0.100E−11	0.128E−08	0.3166E−06
0.316E−12	0.420E−07	0.1312E−06
0.100E−12	0.180E−07	0.1426E−06
0.316E−13	0.286E−07	0.1405E−06
0.100E−13	0.444E−07	0.1086E−06
0.316E−14	0.393E−07	0.1295E−06
0.100E−14	0.206E−07	0.1673E−06
0.316E−15	0.795E−08	0.1872E−06
0.100E−15	0.301E−08	0.1947E−06
0.316E−16	0.421E−08	0.1969E−06
0.100E−16	0.117E−07	0.1963E−06
0.316E−17	0.275E−07	0.1925E−06
0.100E−17	0.432E−07	0.1829E−06
0.316E−18	0.386E−07	0.1675E−06
0.100E−18	0.276E−07	0.1524E−06
0.316E−19	0.607E−07	0.1392E−06
0.100E−19	0.189E−06	0.1182E−06
0.316E−20	0.583E−06	0.3539E−06
0.100E−20	0.171E−05	0.1254E−05

Table 2 Example 1 Noise Level=1.D−8

μ	$\zeta(\mu)$	$\|e(\mu)\|$
0.100E−04	0.244E−03	0.3202E−03
0.316E−05	0.821E−04	0.2955E−03
0.100E−05	0.523E−04	0.4091E−03
0.316E−06	0.765E−04	0.3600E−03
0.100E−06	0.721E−04	0.2115E−03
0.562E−07	0.567E−04	0.1296E−03
0.316E−07	0.398E−04	0.6011E−04
0.178E−07	0.259E−04	0.8939E−05
0.100E−07	0.166E−04	0.2756E−04
0.562E−08	0.131E−04	0.5254E−04
0.316E−08	0.171E−04	0.7223E−04
0.178E−08	0.282E−04	0.9221E−04
0.100E−08	0.476E−04	0.1186E−03
0.316E−09	0.122E−03	0.2251E−03
0.100E−09	0.226E−03	0.4898E−03
0.316E−10	0.246E−03	0.9807E−03

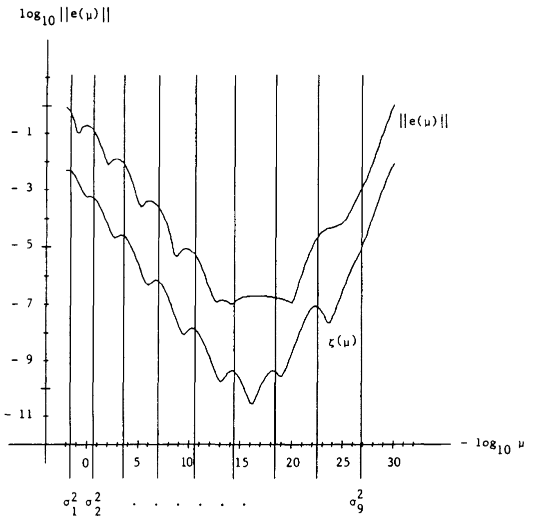

Fig. 1 Example 1 Noise Level=round off.

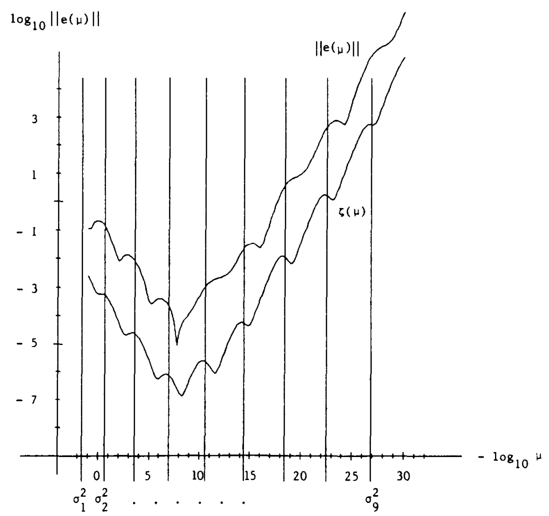

Fig. 2 Example 1 Noise Level=10^{-8}.

about 16 decimal digits (double precison of IEEE standard).

Example 1.

$$\int_0^1 e^{st}\bar{f}(t)\,dt=(e^{s+1}-1)/(s+1), \quad 0\leqq s\leqq 1.0$$

The true solution $\bar{f}(t)=e^t$

$n=19 \quad m=20$

$s_i=0.05i,\ i=1, 2, \ldots, 20,$

$\|T\|=6.0$

Numerical Rank of $T=9$

The computed singular values σ_i, $i=1, 2, \ldots, n$:

$\sigma_1=6.0\times10^{0}$, $\sigma_2=4.7\times10^{-1}$, $\sigma_3=1.6\times10^{-2}$,

$\sigma_4=3.3\times10^{-4}$, $\sigma_5=5.2\times10^{-6}$, $\sigma_6=6.3\times10^{-8}$,

$\sigma_7=6.3\times10^{-10}$, $\sigma_8=5.3\times10^{-13}$, $\sigma_9=3.8\times10^{-14}$.

Singular values from σ_{10} to σ_{19} are numerical zero, or less than $\|T\|\times10^{-16}$.

1-1) Noise level = round off error

$\|e(\mu_0)\|=1.08\times10^{-7}$

$\|e(\mu_\zeta)\|=1.96\times10^{-7}$

Ratio of precision = 0.96

1-2) Noise level $=1.0\times10^{-8}$

$\|e(\mu_0)\|=8.94\times10^{-6}$

Table 3 Example 1 Noise Level = 1.D-4

μ	$\zeta(\mu)$	$\|e(\mu)\|$
0.100E+00	0.383E−01	0.7780E−01
0.582E−01	0.284E−01	0.4484E−01
0.316E−01	0.168E−01	0.2497E−01
0.178E−01	0.102E−01	0.1439E−01
0.100E−01	0.603E−02	0.7860E−02
0.562E−02	0.367E−02	0.8987E−02
0.316E−02	0.277E−02	0.1140E−01
0.178E−02	0.305E−02	0.1181E−01
0.100E−02	0.378E−02	0.1060E−01
0.582E−03	0.430E−02	0.7999E−02
0.316E−03	0.425E−02	0.4373E−02
0.178E−03	0.364E−02	0.3796E−03
0.100E−03	0.280E−02	0.3187E−02
0.562E−04	0.221E−02	0.5721E−02
0.316E−04	0.246E−02	0.6922E−02
0.178E−04	0.388E−02	0.6616E−02
0.100E−04	0.666E−02	0.5136E−02
0.562E−05	0.114E−01	0.6022E−02
0.316E−05	0.191E−01	0.9941E−02
0.178E−05	0.308E−01	0.2466E−01
0.100E−05	0.464E−01	0.5051E−01
0.562E−06	0.637E−01	0.9144E−01

Table 4 Example 2 Noise Level = round off

μ	$\zeta(\mu)$	$\|e(\mu)\|$
0.100E−16	0.351E−05	0.6940E−05
0.562E−17	0.249E−05	0.4734E−05
0.316E−17	0.162E−05	0.3113E−05
0.178E−17	0.998E−08	0.2028E−05
0.100E−17	0.592E−06	0.1350E−05
0.562E−18	0.343E−06	0.9443E−08
0.316E−18	0.196E−06	0.7097E−06
0.178E−18	0.111E−06	0.8120E−08
0.100E−18	0.832E−07	0.5589E−08
0.562E−19	0.368E−07	0.5265E−06
0.316E−19	0.261E−07	0.5107E−06
0.178E−19	0.317E−07	0.5044E−06
0.100E−19	0.530E−07	0.5054E−06
0.562E−20	0.935E−07	0.5139E−06
0.316E−20	0.165E−06	0.5330E−06
0.178E−20	0.292E−06	0.5691E−06
0.100E−20	0.512E−06	0.6536E−06
0.562E−21	0.889E−06	0.8519E−06
0.316E−21	0.152E−05	0.1199E−05
0.178E−21	0.252E−05	0.1800E−05
0.100E−21	0.397E−05	0.2819E−05
0.582E−22	0.583E−05	0.4493E−05
0.316E−22	0.772E−05	0.7174E−05

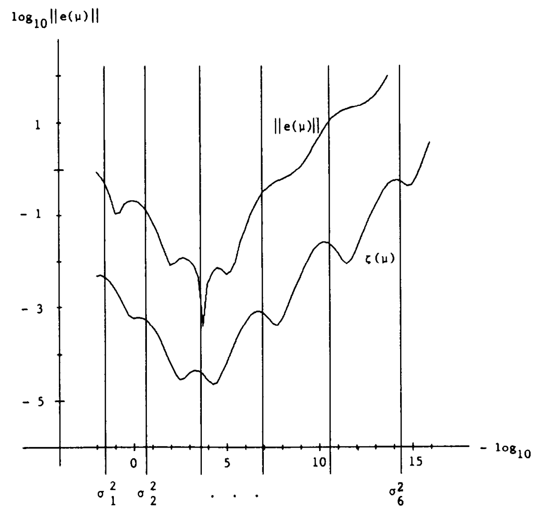

Fig. 3 Example 1 Noise Level $=10^{-4}$.

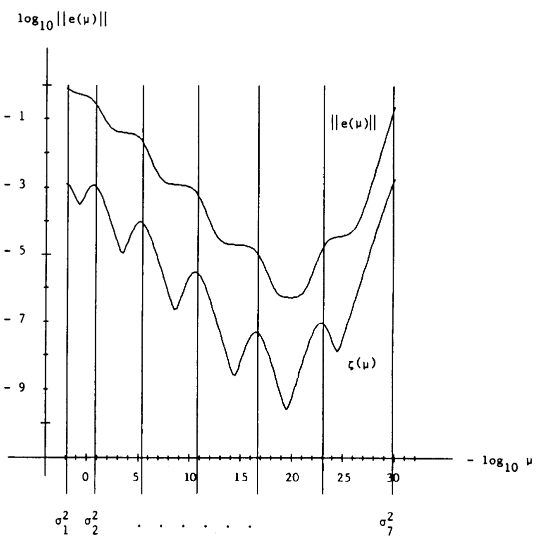

Fig. 4 Example 2 Noise Level = round off.

$\|e(\mu_\zeta)\| = 5.25 \times 10^{-5}$
Ratio of precision $= 0.85$

1-3) Noise level $= 1.0 \times 10^{-4}$
$\|e(\mu_0)\| = 3.80 \times 10^{-4}$
$\|e(\mu_\zeta)\| = 5.72 \times 10^{-3}$
Ratio of precision $= 0.66$

Example 2.

$$\int_0^1 2\cos(st)\bar{f}(t)\,dt = \sin(s+2)/(s+2) + \sin(s-2)/(s-2)$$

$$0 \leqq s \leqq 1.0$$

The true solution $\bar{f}(t) = \cos 2t$
$n = 19$ $m = 20$
$s_i = 0.1(i-1)$, $i = 1, 2, \ldots, 20$,
$\|T\| = 8.5$
Numerical Rank of $T = 7$
The computed singular values σ_i, $i = 1, 2, \ldots, n$:
$\sigma_1 = 8.5 \times 10^0$, $\sigma_2 = 3.8 \times 10^{-1}$, $\sigma_3 = 2.0 \times 10^{-3}$,

Table 5 Example 2 Noise Level = 1.D-8

μ	$\zeta(\mu)$	$\|e(\mu)\|$
0.316E−08	0.247E−04	0.1219E−02
0.100E−08	0.502E−04	0.1181E−02
0.562E−09	0.843E−04	0.1156E−02
0.316E−09	0.137E−03	0.1118E−02
0.178E−09	0.212E−03	0.1058E−02
0.100E−09	0.300E−03	0.9628E−03
0.562E−10	0.379E−03	0.8203E−03
0.316E−10	0.416E−03	0.6270E−03
0.178E−10	0.393E−03	0.3968E−03
0.100E−10	0.321E−03	0.1625E−03
0.562E−11	0.233E−03	0.4090E−04
0.316E−11	0.154E−03	0.1938E−03
0.178E−11	0.965E−04	0.2956E−03
0.100E−11	0.628E−04	0.3560E−03
0.562E−12	0.581E−04	0.3853E−03
0.316E−12	0.871E−04	0.3895E−03
0.178E−12	0.152E−03	0.3689E−03
0.100E−12	0.269E−03	0.3159E−03
0.562E−13	0.478E−03	0.2124E−03
0.316E−13	0.848E−03	0.2163E−03
0.178E−13	0.151E−02	0.3679E−03
0.100E−13	0.267E−02	0.9202E−03

Table 6 Example 2 Noise Level = 1.D-4

μ	$\zeta(\mu)$	$\|e(\mu)\|$
0.316E−01	0.481E−01	0.1216E+00
0.100E−01	0.181E−01	0.6695E−01
0.316E−02	0.608E−02	0.4906E−01
0.100E−02	0.212E−02	0.4213E−01
0.316E−03	0.255E−02	0.3909E−01
0.178E−03	0.424E−02	0.3765E−01
0.100E−03	0.701E−02	0.3565E−01
0.562E−04	0.111E−01	0.3255E−01
0.316E−04	0.164E−01	0.2762E−01
0.178E−04	0.218E−01	0.2004E−01
0.100E−04	0.256E−01	0.9270E−02
0.562E−05	0.258E−01	0.4365E−02
0.316E−05	0.224E−01	0.1927E−01
0.178E−05	0.171E−01	0.3317E−01
0.100E−05	0.117E−01	0.4433E−01
0.582E−08	0.743E−02	0.5229E−01
0.316E−06	0.452E−02	0.5753E−01
0.178E−06	0.277E−02	0.6087E−01
0.100E−06	0.216E−02	0.6308E−01
0.562E−07	0.285E−02	0.6477E−01
0.316E−07	0.486E−02	0.6648E−01
0.178E−07	0.858E−02	0.6677E−01
0.100E−07	0.152E−01	0.7242E−01
0.562E−08	0.269E−01	0.7665E−01
0.316E−08	0.474E−01	0.8956E−01
0.178E−08	0.829E−01	0.1088E+00

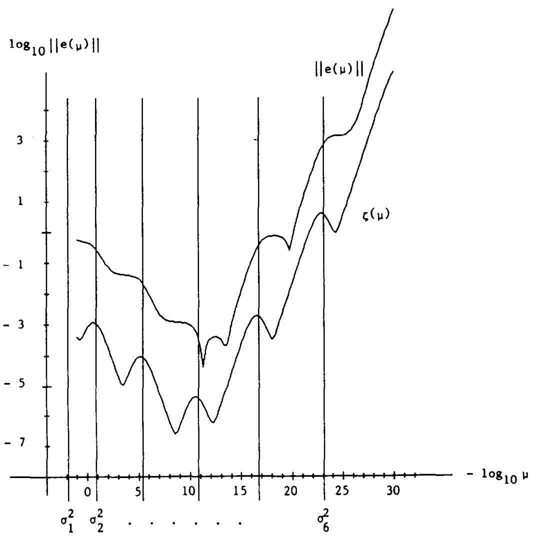

Fig. 5 Example 2 Noise Level $= 10^{-8}$.

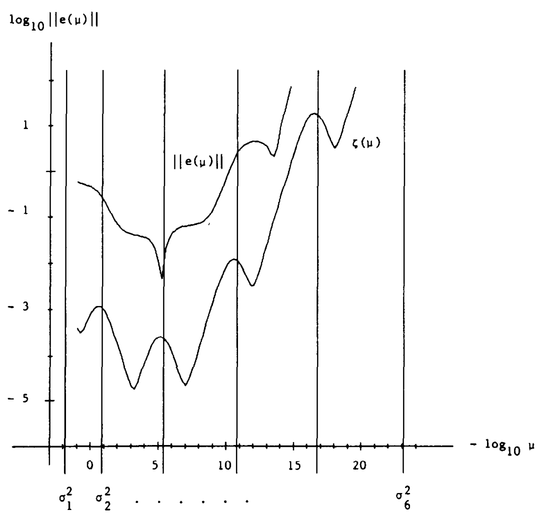

Fig. 6 Example 2 Noise Level $= 10^{-4}$.

$\sigma_4 = 4.1 \times 10^{-6}$, $\sigma_5 = 4.3 \times 10^{-9}$, $\sigma_6 = 2.7 \times 10^{-12}$, $\sigma_7 = 1.2 \times 10^{-15}$.

Singular values from σ_8 to σ_{19} are numerical zero, or less than $\|T\| \times 10^{-16}$.

2-1) Noise level = round off error
$\|e(\mu_0)\| = 5.04 \times 10^{-7}$
$\|e(\mu_\zeta)\| 5.11 \times 10^{-7}$
Ratio of precision = 1.0

2-2) Noise level = 1.0×10^{-8}
$\|e(\mu_0)\| = 5.8 \times 10^{-9}$
$\|e(\mu_\zeta)\| = 1.3 \times 10^{-8}$
Ratio of precision = 0.96

2-3) Noise level = 1.0×10^{-4}
$\|e(\mu_0)\| = 4.37 \times 10^{-3}$
$\|e(\mu_\zeta)\| = 4.04 \times 10^{-2}$
Ratio of precision = 0.59

6. Concluding Remarks

In this paper, we proposed an algorithm to estimate the optimal regularization parameter. Results of the numerical experiments show that the algorithm gives good estimations for wide range of Δg. On the other hand, some statistical approaches are available for this problem of estimating the parameter. Among others, generalized cross validation method is noted for its prominence [5, 8, 11]. A comparison between our algorithm and the method including numerical experiments shall be made elsewhere.

References

1. BABOLIAN, E. and DELVES, L. M. On Augmented Galerkin method for first kind Fredholm integral equations. *J. Inst. Maths. Applics.* **24** (1979), 157-174.
2. ELDEN, L. Algorithms for the regularization of ill-conditioned least squares problems. *BIT* **17** (1977), 134-145.
3. ENGL, H. W. Necessary and sufficient conditions for convergence of regularization methods for solving linear operator equations of the first kind, *Numer. Funct. Anal. Opt.* **3** (1981), 201-222.
4. GOLUB, G. H. and REINSCH, C. Singular value decomposition and least squares solutions, Numer. Math. **14** (1970), 403-420.
5. GOLUB, G. H. HEATH, M. and WAHBA, G. Generalized cross validation as a method for choosing a ridge parameter, *Technometrics*, **21** (1979), 215-223.
6. GOLUB, G. H. and VAN LOAN, C. F. Matrix Computations, The John Hopkins University Press. 1983.
7. GROETSCH, C. W. Generalized Inverse of Linear Operators, Marcel Dekker, 1977.
8. GROETSCH, C. W. The Theory of Tikhonov Regularization for Fredholm Equations of the First Kind, pitman 1984.
9. HAMMERLIN, G. et al. eds, Improperly Posed Problems and their Numerical Treatment, Birkhauser, 1983.
10. HANSON, R. J. A Numerical method for solving Fredholm integral equation of the first kind using singular values, *SIAM J. Num. Anal.* **8** (1971), 616-622.
11. HILGERSJ. W. On the equivalence of regularization and certain reproducing kernel Hilbert space approaches for solving first kind problems, *SIAM J. Num. Anal.* **13** (1976), 172-184.
12. KITAGAWA, T. A deterministic approach to the optimal regularizaiton, *Japan J. of Appl. Math.* **4** (1987), 371-391.
13. Lintz, P. Uncertainty in the solution of linear operator equations, *BIT* **24** (1984), 172-184.
14. NASHED, M. Z. ed. Generalized Inverses and Applications, New York, Academic, 1976.
15. NASHED, M. Z. Operator theoretic and computational approaches to ill-posed problems with applications to antenna theory, *IEEE Trans. Antennas Propagat.* **29** (1981), 220-231.
16. PRENTER, P. M. Splines and Variational Methods, John Wiley & Sons Inc., New York (1975).
17. TIKHONOV, A. N. and ARSENIN, V. W. Solutions of Ill-Posed Problems. Winston-Wiley New York, 1977.
18. VARAH, J. M. Pitfalls in the numerical solution of linear ill-posed problems, *SIAM J. Sci. Stat. Comput.* **4** (1983), 164-176.
19. VOEVODIN, V. V. The method of regularization. *Zh. Vychsl. Mat. Mat. Fiz.* **9** (1969), 673-675.
20. WAHBA, G. Practical approximate solutions to linear operator equations when the data are noisy, *SIAM J. Numer. Anal.* **14** (1977), 651-667.

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