,

Tikhonov regularization in general form with Chebfun

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Linear ill-posed problems often are analyzed in function spaces using tools from functional analysis, while their numerical solution typically is computed by first discretizing the problem and then applying tools from finite-dimensional linear algebra. The Chebfun package makes it possible to solve linear ill-posed problems without explicit discretization. This work discusses the use of Tikhonov regularization with a fairly general linear regularization operator within the Chebfun framework.

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1 Introduction

We are interested in determining an approximate solution of least-squares problems of the form

$$\min_{x\in L^2(\Omega_1)} \left\| \int_{\Omega_1} \kappa(s,t)x(t)\,dt - g^\delta(s) \right\|_{\Omega_2}, \tag{1}$$

where Ω_i is a subset of $\mathbb{R}^{d_i}$ equipped with the standard L_2-norm and d_i is a small positive integer for $i \in \{1,2\}$. The kernel κ is assumed to be square integrable and the function g^δ represents available data that are contaminated by measurement error. This kind of problems arise in numerous applications including remote sensing, fluid mechanics, signal processing, and image restoration.

Let $g_{\rm exact}$ denote the unavailable error-free function that is associated with g^δ and let $x_{\rm exact}$ denote the solution of minimal norm of

$$\int_{\Omega_1} \kappa(s,t)x(t)\,dt = g_{\rm exact}(s), \qquad s \in \Omega_2, \tag{2}$$

where we tacitly assume that the above equation is consistent. This is required in order to be able to apply the discrepancy principle to determine a regularization parameter introduced below. If equation (2) is not consistent, then the discrepancy principle should not be used; we will comment on this situation below.

We are interested in determining an accurate approximation of $x_{\rm exact}$ when only an approximation g^δ of the function $g_{\rm exact}$ is known. The approximation of $x_{\rm exact}$ is computed by determining a suitable approximate solution of (1).

A frequently used example of equation (1) that arises in image restoration is when the kernel models Gaussian blur, that is when

$$\kappa(s,t) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(\frac{(s-t)^2}{2\sigma^2} \right). \tag{3}$$

Then $\Omega_1 = \Omega_2$ are rectangles in the plane, and the solution $x(t)$, $t \in \Omega_1$, of (1) represents a grayscale image. The kernel models the blurring of the unavailable exact grayscale image that is represented by $x_{\rm exact}(t)$, $t \in \Omega_1$, and which we would like to determine. In this application, the kernel often is referred to as a point-spread function. In particular, the parameter $\sigma > 0$ determines how much the image is blurred. The function $g^\delta(s)$, $s \in \Omega_2$, represents an available blurred and noisy image, while $g_{\rm exact}(s)$, $s \in \Omega_2$, defined by (2) with $x(t) = x_{\rm exact}(t)$ represents an unavailable blurred, but noise-free image. The difference $g^\delta - g_{\rm exact}$ models the noise in the available image g^δ. In many image restoration applications, the noise is white Gaussian. Note that κ is smooth; in particular κ is square integrable. The computation of an approximation of the exact image $x_{\rm exact}$ by determining an approximate solution of (1) is commonly referred to as *deconvolution*.

Straightforward solution of (1) generally yields a poor approximation of $x_{\rm exact}$ due to significant propagation of the noise in g^δ into the computed solution. To discuss how an accurate approximation of $x_{\rm exact}$ can be computed, it is convenient to define the integral operator

$$(Ax)(s) = \int_{\Omega_1} \kappa(s,t)x(t)\,dt.$$

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Due to the fact that κ is square integrable, the integral operator does not have a bounded inverse. This follows from the Riemann-Lebesgue lemma, which shows that $A\cos(2\pi mt)$ is arbitrarily small for m sufficiently large. However, the maximum of $|\cos(2\pi mt)|$ for $0 \leq t \leq 1$ is 1. This result indicates that small perturbations (e.g., errors) in the data function g^δ may give rise to large changes in the computed solution of (1). This makes the solution of (1) a so-called ill-posed problem; see [9, 15] for details on the Riemann-Lebesgue lemma and its ramification.

Tikhonov regularization [28] aims to reduce the sensitivity of the solution of (1) to the noise in g^δ by replacing the minimization problem (1) by the penalized least-squares problem

$$\min_{x\in L^2(\Omega_1)} \left\{ \left\| Ax - g^\delta \right\|_{\Omega_2}^2 + \mu \|Lx\|_{\Omega_1}^2 \right\}, \tag{4}$$

where L is a linear regularization operator and $\mu > 0$ is a regularization parameter. This parameter balances the relative influence of the two terms in (4).

We will consider the situation when L is a differential operator chosen so that the null spaces of A and L intersect trivially. Then (4) has a unique solution x_μ for any $\mu > 0$; see [15]. The Tikhonov regularization problem (4) is said to be in *standard form* when L is a multiple of the identity; otherwise, the problem is in *general form*.

There are several approaches to determine a suitable value of μ; see, e.g., [9, 15, 19, 20, 26, 27]. They typically require the solution of (4) for several μ-values. For instance, when the *discrepancy principle* is used to determine μ, one seeks to find the unique value of $\mu > 0$ so that the solution x_μ of (4) satisfies

$$\left\| Ax_\mu - g^\delta \right\|_{\Omega_2}^2 = \eta^2\delta^2, \tag{5}$$

where δ is an upper bound for the norm of the error $\|g_{\rm exact} - g^\delta\|_{\Omega_2}$, which is assumed to be available, and $\eta > 1$ is a user-specified parameter that is independent of δ; see [9]. The solution of (5) for $\mu > 0$ (which determines x_μ) requires a zero-finder and the repeated solution of (4) for different μ-values. We will use the discrepancy principle in the computed examples presented below.

Another popular method for determining a suitable value of $\mu > 0$ is furnished by the *L-curve criterion*. This criterion seeks to determine the point on the curve

$$\mu \to \left(\ln \left\| Ax_\mu - g^\delta \right\|_{\Omega_2}, \ln \|Lx_\mu\|_{\Omega_1} \right), \qquad \mu_{\min} \leq \mu \leq \mu_{\max},$$

with largest curvature. This requires the solution of (4) for several values of μ. The curve obtained typically is L-shaped with the "corner" of the "L" corresponding to a suitable value of μ; see [4, 17] for further details. The determination of an fairly accurate location of the "corner" generally requires that the minimization problem (4) be solved for several μ-values. We hasten to add that this approach of determining a suitable value of μ often gives useful results, but may fail to do so for some problems; see Kindermann [19] for a discussion. But we note that when equation (2) does not hold, i.e., when $g_{\rm exact}$ is not in the range of the operator A, the discrepancy principle should not be used to determine μ. In this situation other techniques, such as the L-curve criterion, generalized cross validation, or the method described by Park et al. [26] can be employed.

The standard way of solving (4) is to first discretize the operators A and L, and then compute the generalized singular value decomposition (GSVD) of the pair of matrices so obtained; see, e.g., [8, 13, 15] for a description of this approach. Having computed the GSVD, the left-hand side of (5) can be evaluated quite rapidly for different μ-values.

Solving Tikhonov regularization problems in general form is more costly than the solution of Tikhonov regularization problems in standard form. However, the extra flexibility provided by using an operator L different from the identity often gives computed approximations of $x_{\rm exact}$ of higher quality. In the standard form problem, the solution x_μ is pushed towards 0, while the solution of a problem in general form with L a differential operator pushes the solution towards being smooth. Generally, the regularization operator L should be chosen so that known important features of the desired solution $x_{\rm exact}$ are not damped. For instance, if $x_{\rm exact}(t)$ is known to be an increasing real-value function of a real variable t, then it may be appropriate to let L be a second order differential operator, say $L = d^2/dt^2$, whose nullspace include constant and linear functions. In the continuous setting, the most common regularization operators different from the identity are differential operators [9, 12]; in the discrete setting many techniques for constructing suitable regularization matrices have been proposed. Their construction uses finite difference approximations of derivatives [5, 11, 15, 21], orthogonal projections [22], reordering of the unknowns [3, 25], the solution of minimization problems [7, 24], and the solution of an inverse problem [23].

We are interested in solving (4) by using the MATLAB package Chebfun [6]. This package approximates functions by piece-wise polynomials anchored at translated Chebyshev points. These piece-wise polynomials are referred to as *chebfuns*. All computations within Chebfun's framework are carried out with these approximations of actual functions. A user does not explicitly have to choose how to define the chebfuns; this is done by the Chebfun package. In particular, a user can work with (approximations of) functions and operators without initial explicit discretization. Illustrations of the solution of minimization problems (4) in standard form when using Chebfun can be found in [1]. The main advantage of applying Chebfun, when compared to the standard solution approach of discretizing the equation (4) first, is that it allows a user to carry out the computations in a way that feels closer to the theory for ill-posed problems. In particular, a user does not have to choose a

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suitable discretization before starting to solve the problem. This is advantageous, because it is not always straightforward to determine how fine the discretization should be chosen. We note that using a discretization that is unnecessarily fine makes the solution process needlessly expensive. Computed examples reported in [1] illustrate that discretization first may for some problems require more CPU time than the regularization first approach implemented with Chebfun. The regularization first approach provides us with suitable ansatz functions for the discretization and makes the subsequent discretization simpler. However, we should mention that Chebfun only simulates the regularization first approach, since the approximation by piecewise polynomials employed by Chebfun itself is a form of discretization. Thus in the end we replace the standard solution approach

$$\text{Discretization} \rightarrow \text{Regularization}$$

by

$$\text{Hidden discretization by replacing } f \text{ by a chebfun} \rightarrow \text{Regularization} \rightarrow \text{Discretization.}$$

The last discretization stems from the fact that the computed solution is expressed in terms of a finite sum of functions, each of which is represented by a chebfun. It is important to note that when using Chebfun, a user does not have to explicitly discretize the problem; all discretizations are furnished by Chebfun. This lends a user of Chebfun the impression of working with functions and operators.

This work is concerned with the solution of (4) in general form. A difficulty to overcome is that Chebfun, at least for now, does not have an implementation of an analogue of the GSVD.

2 A solution method

Chebfun can be applied to compute the singular value expansion of the kernel

$$\kappa(s,t) = \sum_{i=1}^{\ell} \sigma_i \phi_i(s) \psi_i(t),$$

where the singular functions $\{\phi_i\}_{i=1}^{\ell}$ are orthogonal in Ω_2, the singular functions $\{\psi_i\}_{i=1}^{\ell}$ are orthogonal in Ω_1, and the number of terms, ℓ, is determined by Chebfun. Details on how Chebfun computes the singular value expansion can be found in [29]. Typically, $\ell \leq 100$; see [1] for illustrations.[1] We seek to determine an approximate solution of (4) of the form

$$x(t) = \sum_{i=1}^{\ell} \beta_i \psi_i(t). \tag{6}$$

That is, we are using the span of the singular functions $\{\psi_i\}_{i=1}^{\ell}$ as ansatz space for the solution of the problem (1). The coefficients β_i are determined by the function g^{δ} in (1). We ignore solution components that cannot be represented by the expansion (6).

For definiteness, let Ω_1 and Ω_2 be bounded intervals on the real axis and let L be the second derivative operator. Substituting (6) into (4), and using the fact that standard L_2 norms are used, gives

$$\min_{\beta} \left\{ \int_{\Omega_2} \left| \int_{\Omega_1} k(s,t) \left(\sum_{j=1}^{\ell} \beta_j \psi_j(t) \right) dt - g^{\delta} \right|^2 ds + \mu \int_{\Omega_1} \left| \sum_{j=1}^{\ell} \beta_j L\psi_j(t) \right|^2 dt \right\}, \tag{7}$$

where $\beta = [\beta_1, \ldots, \beta_\ell]^T$. The functions $\psi_j^{(2)}(t) = L\psi_j(t)$ easily can be computed with the Chebfun command `diff`, which computes the derivative of a function. Note that the functions $\psi_j^{(2)}(t)$ do not form an orthogonal set. We obtain from (7) the new minimization problem

$$\min_{\beta} \left\{ \sum_{i=1}^{\ell} \beta_i^2 \sigma_i^2 - 2 \sum_{i=1}^{\ell} \beta_i \sigma_i \int_{\Omega_2} \phi_i(s) g^{\delta}(s)\, ds + \int_{\Omega_2} \left| g^{\delta} \right|^2 ds + \mu \sum_{i=1}^{\ell} \sum_{j=1}^{\ell} \beta_i \beta_j \int_{\Omega_1} \psi_i^{(2)}(t) \psi_j^{(2)}(t)\, dt \right\}.$$

[1] Chebfun only computes a truncated approximation of the singular value expansion with a tolerance chosen by the user, we choose 10^{-16}. Thus, within the computation of the singular value expansion lies another hidden regularization known as truncated SVD (TSVD); see [14] for details.

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We will use matrix notation to simplify this problem. Define

$$\Sigma = \mathrm{diag}[\sigma_1, \ldots, \sigma_\ell] \in \mathbb{R}^{\ell\times\ell},$$
$$g_\phi^\delta = [g_{\phi,i}^\delta]_{i=1}^\ell, \quad g_{\phi,i}^\delta = \sigma_i \int_{\Omega_2} \phi_i(s) g^\delta(s)\, ds,$$
$$\Psi = [\Psi_{ij}]_{i,j=1}^\ell, \quad \Psi_{ij} = \int_{\Omega_1} L\psi_i(t) L\psi_j(t)\, dt.$$

Then the minimization problem (7) can be written as

$$\min_\beta \Big\{ \beta^T \Sigma^2 \beta - 2\beta^T g_\phi^\delta + \mu \beta^T \Psi \beta \Big\}.$$

Its minimum is the solution of the linear system of equations

$$\left(\mu\Psi + \Sigma^2\right)\beta = g_\phi^\delta. \tag{8}$$

This system has to be solved repeatedly to determine a value of μ such that the associated solution x_μ satisfies (5); the sequence of the computed μ-values are determined by a zero-finder, such as Newton's method, applied to equation (5). The matrix $\mu\Psi + \Sigma^2$ is symmetric positive definite for any $\mu > 0$. Moreover, this matrix is not very large. Therefore, we can solve the system repeatedly for different μ-values by Cholesky factorization of the matrix in (8); we remark that each new μ-value requires that a new Cholesky factorization be computed. Alternatively, we can compute the GSVD of the matrix pair $\{\Psi, \Sigma^2\}$. With the latter decomposition available, it is inexpensive to solve the system (8) repeatedly for several μ-values.

3 Model problems and numerical experiments

We present two computed examples that illustrate the performance of the method described above. The first computed example is an integral equation (1) with

$$\kappa(s,t) = \sqrt{s^2 + t^2}, \qquad g_{\mathrm{exact}}(s) = \frac{1}{3}((1+s^2)^{3/2} - s^3),$$

and solution $x_{\mathrm{exact}}(t) = t$. Here $\Omega_1 = \Omega_2 = [0,1]$. This example was first used by Fox and Goodwin [10]. The other example is an integral equation (1) defined by

$$\kappa(s,t) = \frac{d}{(d^2 + (st)^2)^{3/2}}$$

with $d = 0.25$ and $\Omega_1 = \Omega_2 = [0,1]$. The solution $x_{\mathrm{exact}}(t) = \sin(\pi t) + 0.5\sin(2\pi t)$ is given and defines the right-hand side function $g_{\mathrm{exact}}(s)$ by (2). This problem is described in [30]; it is often referred to as `gravity`; see, for instance, [16].

The functions g_{exact} in the examples are assumed not to be known, but associated error-contaminated functions g^δ, defined by

$$g^\delta = g_{\mathrm{exact}}(s) + \delta \frac{\|g_{\mathrm{exact}}(s)\|_{\Omega_2}}{\|F(s)\|_{\Omega_2}} F(s),$$

are assumed to be available. Here the function $F(s)$ is a smooth Chebfun function, generated with the Chebfun command `randnfun(`ϑ`,`Ω_2`)`, with maximum frequency about $2\pi/\vartheta$ and standard normal distribution $N(0,1)$ at each point. The parameter $\delta > 0$ specifies the noise level. In the computed examples, we let $\vartheta = 10^{-2}$.

Figures 1 and 2 display the computed solutions $x_\mu(t)$ as well as the desired solutions $x_{\mathrm{exact}}(t)$ for the test problems with L being the differential operator d^2/dt^2. The computed solutions can be seen to be very close to the desired solution for both test problems. When, instead, L is the identity operator, the computed solutions are less close to $x_{\mathrm{exact}}(t)$. This is illustrated in Figure 3, which compares the quality of the computed approximations $x_\mu(t)$ of $x_{\mathrm{exact}}(t)$ determined by Tikhonov regularization in both standard and general forms. The accuracy of the computed approximate solution $x_\mu(t)$ is measured by the relative error

$$RE = \frac{\|x_{\mathrm{exact}}(t) - x_\mu(t)\|_{\Omega_1}}{\|x_{\mathrm{exact}}(t)\|_{\Omega_1}}. \tag{9}$$

Figure 3 shows that the use of the second derivative operator instead of the identity operator can improve the quality of the computed approximate solutions significantly.

We finally note that Chebfun performs the best when Ω_1 and Ω_2 are intervals. It is possible to apply Chebfun when the sets Ω_i are rectangles and the kernel has special structure. This is illustrated in [1]; see below for comments on the limitations of Chebfun.

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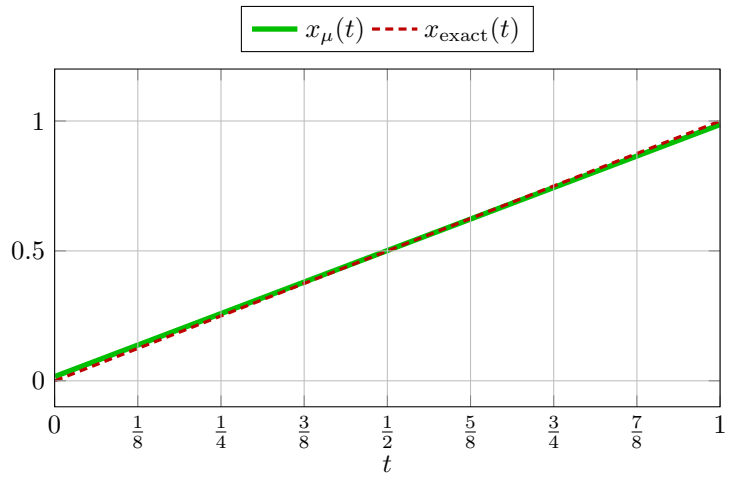

Fig. 1: Example—"`Fox-Goodwin`", $\delta = 1.00\,\text{e}{-2}$.

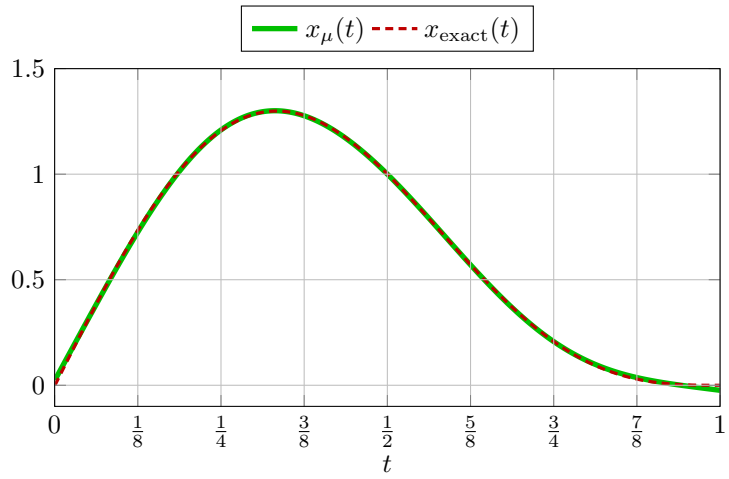

Fig. 2: Example—"`Gravity`", $\delta = 1.00\,\text{e}{-3}$.

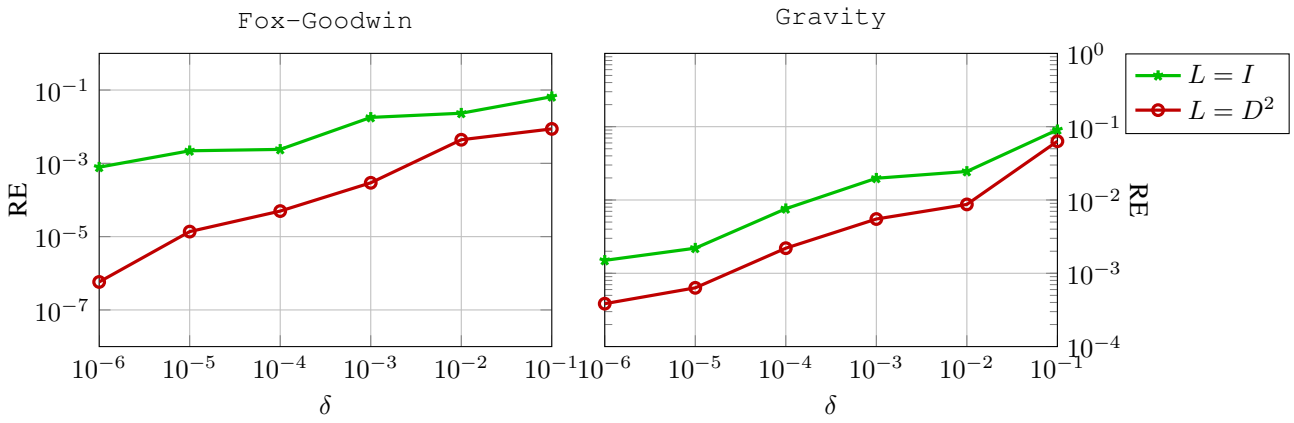

Fig. 3: Comparison of the quality of the computed solutions by Tikhonov regularization in standard and general forms. The green stars represent the relative error when Tikhonov regularization is applied with L as the identity for different values of level noise δ. The red circles represent the relative error when Tikhonov regularization is applied with L as the second derivative for different values of level noise δ.

4 Conclusions and extensions

In this short paper we discussed the solution of Tikhonov regularization in general form with the aid of Chebfun. The numerical experiments illustrate that this approach is capable of computing accurate approximations of the desired exact solution x_{exact} of ill-posed problems despite the fact that the available data function g^δ is contaminated by error. The examples show that the quality of the computed solutions x_μ can be much higher when L is a differential operator than when L is the identity. This

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has been illustrated in the literature before both in infinite-dimensional and finite-dimensional settings, and is the reason for our interest in Tikhonov regularization in general form.

The approach described in this paper is restricted by two limitations of Chebfun. Currently it is not possible to compute a GSVD with Chebfun. It is our understanding that at least for two-dimensional kernel functions it is possible to add a GSVD function to Chebfun with limited effort. Secondly, it is currently not possible to use Chebfun when the kernel function is a general function in four or six dimensions. Such kernel functions arise necessarily for two- and three-dimensional domains Ω_i. This limitation is harder to overcome and we do not expect Chebfun to include such capabilities anytime soon. The latest extension, called Chebfun3 [18], introduced three dimensional Chebfuns.

There is a package similar to Chebfun for Julia called ApproxFun [2]. It may be possible to overcome some of Chebfun's limitation within the framework of ApproxFun. We plan to investigate this.

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