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On Ill-Conditioned Linear Systems and Regularized GMRES Method

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In this paper we consider solving ill-conditioned square linear systems with noisy right hand sides. To have meaningful solutions of such systems, we use Tikhonov regularization with the GMRES method in three different ways. Our computational experiments show that solving the noisy system by regularizing the least square problem inside the GMRES algorithm gives us meaningful solutions and is much faster than regularizing the original least square model itself or its least square problem within the GMRES method.

Keywords: Ill-conditioned linear systems, GMRES method, Tikhonov regularization.

1 Introduction

Ill-conditioned linear systems frequently arise in many real world applications [3, 5]. Solving such systems are of great interests for many years and various approaches have been developed to do so. In this paper we deal with the following kind of ill-conditioned linear systems:

$$Ax = b, \tag{1.1}$$

where A is a square ill-conditioned matrix. Therefore, a slight perturbation in vector b might significantly change the solution norm. For example, let us consider problem 'heat' from the regularization tools [5] with $n = 1000$, $||x_s|| = 0.5779$ (x_s is the exact solution) and perturb the right hand vector as $b_0 = b + 1e - 3 * rand(1000, 1)$. Then the computed solution by MATLAB backslash command is $7.9689e + 019$ with $||Ax - b_0|| = 1.2009$ and $||Ax - b|| = 1.1999$, and by brute force GMRES is $5.2250e + 009$ with $||Ax - b_0|| = 0.0303$ and $||Ax - b|| = 0.0028$. As we see, this slight perturbation results to a huge change in the solution norm for both methods. We also know that GMRES method is one of the widely used iterative methods and having problem with this ill-conditioned system.

For the rest of the paper, we suppose that the original right hand side is not at hand and let us denote the noisy right hand side by b_0. Thus the system we deal with throughout the paper is

$$Ax = b_0. \tag{1.2}$$

Various approaches have been utilized to deal with such noisy ill-conditioned systems with the iterative methods. For example, a very famous and effective approach is the so called Tikhonov regularization, which has been widely used in the literature [3, 5, 9, 12]. In the Tikhonov regularization, one deals with the following minimization problem

$$\min_x ||Ax - b_0||^2 + \rho^2||x||^2, \tag{1.3}$$

where ρ is the so called regularization parameter. The exact value of ρ is not known in prior, and several strategies have been proposed for selecting the regularization parameter, like the Morozov [10] and Mallows [8] criteria, the Generalized Cross Validation (GCV) [2] and the L-curve method [4]. In [1] the authors have presented a numerical scheme for Tikhonov regularization of ill-conditioned linear systems based on Lancosz bidiagonalization and Gauss quadrature. In their work, they assume that an estimate of the norm of error is available. This allows them to determine the regularization parameter using the discrepancy principle. Truncated SVD (TSVD) is another commonly used method of regularization of ill-conditioned linear systems. The idea of TSVD has been treated as a problem of determining the numerical rank of the matrix A. All of the computed singular values smaller than some threshold value are treated as zeros which were corrupted by rounding errors into small non-zero quantities [6, 7, 9].

Obviously (1.3) is a strictly convex minimization problem and the necessary and sufficient optimality condition is

$$(A^T A + \rho^2 I)x = A^T b_0. \tag{1.4}$$

Now (1.4) can be solved using any iterative methods like GMRES and conjugate gradient methods.

In this article, we use Tikhonov regularization technique in three different ways by the GMRES method. First we solve system (1.4) using GMRES method. In the second case, we consider the least square model of (1.2), but regularize the least square problem within the GMRES method. Finally, we consider the noisy linear system (1.2) and regularize the least square problem within the GMRES method. Our computational results show that the last approach generates meaningful solutions in much faster time than the first two approaches and even better than the conjugate gradient method.

2 GMRES Method

In this section we briefly describe the GMRES method [11]. The GMRES method is an important iterative method for solving linear systems such as (1.2). It starts with an initial guess of the solution, then generates approximate solutions from the affine subspace $x_0 + K_m(A, r_0)$ which minimizes the Euclidean norm of the residual

$$||b_0 - Ax_k|| = \min_{x \in x_0 + K_m(A,r_0)} ||b_0 - Ax||,$$

where $r_0 = b_0 - Ax_0$ is the initial residual and $K_m(A, r_0)$ is the Krylov subspace generated by A, r_0 as

$$K_m(A, r_0) = span\{r_0, Ar_0, \ldots, A^{m-1}r_0\}.$$

The GMRES method is based on the Arnoldi process which constructs an orthonormal basis of Krylov subspace $K_m(A, r_0)$. First we present this algorithm, which uses the modified Gram-Schmidt process.

Algorithm 1: Arnoldi process (Gram-Schmidt process)

Step 1: Choose a vector v_1 such that $||v_1|| = 1$ and an integer $m \leq n$.
Step 2: For $k = 1, \ldots, m$ do
$v_{k+1} = Av_k$,
For $i = 1, \ldots, k$ do
$h_{i,k} = (v_{k+1})^T v_i$,
$v_{k+1} = v_{k+1} - h_{ik}v_i$.
end
$h_{k+1,k} = ||v_{k+1}||$.
$v_{k+1} = v_{k+1}/h_{k+1,k}$.
end

Now let the matrix $\bar{H}_m$ be the upper Hessenberg matrix whose nonzero entries are the scalars h_{ij} and V_m denotes the $n \times m$ matrix whose columns are the elements of the orthogonal $\{v_1, \ldots, v_m\}$ basis constructed by the Algorithm 1. From Arnoldi process, it follows that

$$AV_m = V_{m+1}\bar{H}_m. \tag{2.1}$$

Now we would like to solve the least-squares problem

$$\min_{x \in K_m(A,r_0)} ||b_0 - A(x_0 + x)|| = \min_{x \in K_m(A,r_0)} ||r_0 - Ax||. \tag{2.2}$$

If we set $x = V_m y$, then (2.2) is equivalent to minimize the following function

$$\min_{y \in R^m} ||\beta v_1 - AV_m y||,$$

where we set $\beta = ||r_0||$ for convenience. From (2.1) we have that

$$||\beta v_1 - AV_m y|| = ||V_{m+1}(\beta e_1 - \bar{H}_m y)|| = ||\beta e_1 - \bar{H}_m y||.$$

The last equality follows from the fact that V_{k+1} is an orthonormal matrix. Therefore, it is sufficient to solve the following problem instead of (2.2):

$$\min_{y \in R^m} ||\beta e_1 - \bar{H}_m y||. \tag{2.3}$$

Now the GMRES algorithm can be outlined as follows:

Algorithm 2: Generalized minimal residual(GMRES) method

Step 1: Choose a starting point $x_0 \in R^n$ and a dimension m of Krylov subspace. Compute $r_0 = b_0 - Ax_0$ and $v_1 = r_0/||r_0||$.

Step 2: Perform m steps of Algorithm 1 to generate matrix $\bar{H}_m$ and the orthogonal matrix V_m.

Step 3: Form the approximate solution: $x_k = x_0 + V_m y_m$, where y_m minimizes (2.3).

3 Tikhonov Regularization and GMRES Method

As we see from the previous section, one should solve least square problems within the GMRES method. Therefore, we either can regularize the original least square problem or regularize the least square problem within the GMRES method. Thus we consider the following cases:

- In the first approach, we solve (1.4) using GMRES and conjugate gradient methods.
- In the second approach, we consider the least square problem without any regularization term and regularize the least square problem within the GMRES algorithm. Namely, the GMRES method is applied to the system

$$A^T A x = A^T b_0, \tag{3.1}$$

  while the following regularized least square problem is solved within the GMRES method:

$$\min_{y_m \in R^m} ||\bar{H}_m y_m - \beta e_1||^2 + \rho^2 ||y_m||^2. \tag{3.2}$$

- Finally, in the third approach instead of the least squares problem, we consider the noisy system (1.2). Then we apply the GMRES method to this system, while using the regularized least square problem within the GMRES method. Obviously the computational cost of this approach is much less than the previous two approaches. Therefore, if this approach generates meaningful solutions, then it seems to be the right choice for dealing with noisy ill-conditioned linear systems.

Table 4.1: Comparison of Variants of GMRES method and Conjugate Gradient method

problem	$\|\|Ax^{*}-b\|\|$	$\|\|x\|\|$	time (sec)
baart-1000 $\|\|x_s\|\| = 1.2533$	$(0.0162, 0.0177, 0.0162, 0.0162)$	$(1.2469, 1.2455, 1.2469, 1.2469)$	(1.03,1.78,0.87,1.08)
baart-2000 $\|\|x_s\|\| = 1.2533$	$(0.0224, 0.0234, 0.0224, 0.0224)$	$(1.2549, 1.2510, 1.2549, 1.2549)$	(7.37,9.79,2.72,7.6)
baart-3000 $\|\|x_s\|\| = 1.2533$	$(0.0279, 0.0289, 0.0279, 0.0289)$	$(1.2565, 1.2581, 1.2565, 1.2565)$	(23.83,27.87,4.82,24.3)
heat-1000 $\|\|x_s\|\| = 7.7829$	$(0.016, 0.1364, 0.0157, 0.016)$	$(7.7003, 5.8370, 7.7523, 7.7003)$	(1.14,1.75,0.88,1.4)
heat-2000 $\|\|x_s\|\| = 11.0066$	$(0.0215, 0.1931, 0.0212, 0.0215)$	$(10.8661, 8.2452, 10.9546, 10.8661)$	(7.82,9.5,2.68,8.7)
heat-3000 $\|\|x_s\|\| = 13.4803$	$(0.0271, 0.2367, 0.0267, 0.0271)$	$(13.3142, 10.0982, 13.4191, 13.3142)$	(26.1,27.5,4.83,26.35)
shaw-1000 $\|\|x_s\|\| = 31.5659$	$(0.0149, 0.1383, 0.0149, 0.0149)$	$(31.5554, 32.211, 32.9995, 31.5554)$	(1.08,1.8,0.88,1.11)
shaw-2000 $\|\|x_s\|\| = 44.6410$	$(0.0218, 0.1956, 0.0219, 0.0218)$	$(44.6277, 45.7482, 46.823, 44.6277)$	(7.4,9.46,2.58,7.7)
shaw-3000 $\|\|x_s\|\| = 54.6738$	$(0.0263, 0.2396, 0.0263, 0.0263)$	$(54.6547, 56.6570, 57.2693, 54.6547)$	(24.05,27.6,4.8,24.73)
wing-1000 $\|\|x_s\|\| = 0.5779$	$(0.0155, 0.0181, 0.5389, 0.0155)$	$(0.5215, 0.3755, 0.5779, 0.5215)$	(1.14,1.7,1.14,1.05)
wing-2000 $\|\|x_s\|\| = 0.5771$	$(0.0223, 0.0239, 0.0223, 0.0223)$	$(0.5668, 0.3950, 0.5870, 0.5668)$	(8.02,9.8,2.7,7.4)
wing-3000 $\|\|x_s\|\| = 0.5774$	$(0.0275, 0.0287, 0.0275, 0.0275)$	$(0.5909, 0.4075, 0.6136, 0.5909)$	(23.7,27.7,5,24)

4 Computational Experiments

In this section we present several examples showing the computational behavior of the discussed approaches and the conjugate gradient method. Test problems are taken from [5]. For all algorithms we use the regularization parameter equal to $1e-5$, however it should be noted again that a desired value can be obtained using the L-curve method. Our experiments are done on a Pentium 4 laptop with 1GBs of RAM using MATLAB 7.1. The order of numbers in parenthesis in Table 4.1 are the first, the second, the third, and the conjugate gradient approaches. Our computational experiments show that solving the system $Ax = b_0$ using the regularized GMRES method give meaningful solutions like the other approaches in much shorter time.

5 Conclusions

In this article, we have considered singular square linear systems that are very sensitive to slight perturbation in problem data. To have meaningful solutions of such systems, we have used the Tikhonov regularization technique in three different ways by the GMRES and conjugate gradient methods. Our computational results show that solving the noisy systems by using the regularization within the GMRES method generates meaningful solutions like the other methods in much shorter time.

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