PRIMER FOR THE MATLAB FUNCTIONS
RRGMRES_ITER, RRGMRES_DP, SYM_RRGMRES_ITER & SYM_RRGMRES_DP

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1. Introduction. This primer describes four MATLAB functions for the iterative solution of large linear discrete ill-posed problems,

$$Ax = b, \qquad A \in \mathbb{R}^{m\times m}, \qquad x, b \in \mathbb{R}^m, \tag{1.1}$$

with an error-contaminated right-hand side b. The functions `rrgmres_iter` and `rrgmres_dp` are for problems with a (square) nonsymmetric matrix, and the functions `sym_rrgmres_iter` and `sym_rrgmres_dp` are for the solution of large symmetric problems. The iterative methods implemented by these functions are described in [6, 7], where also several properties of these methods are discussed. The primer also describes several auxiliary MATLAB functions.

2. Files and installation. The file *rrgmres.zip*, which is available from NETLIB at

http://www.netlib.org/numeralgo/naXX,

contains this primer as well as the files listed in Table 2.1. All files should be extracted and placed in the same directory before use. The code has been developed and tested using MATLAB version 7.11 (R2010b) by MathWorks. No other MathWorks products or toolboxes are required. To use all features of the demos, certain test problems from the MATLAB package Regularization Tools by Hansen [3] should be available. These functions are freely available on the Internet; see *http://www2.imm.dtu.dk/∼pch/Regutools/index.html*

3. Input parameters for and output from `rrgmres_iter`, `rrgmres_dp`, `sym_rrgmres_iter`, and `sym_rrgmres_dp`. These functions require specific input parameters. Table 3.1 displays the syntax for input parameters and for the output for each function. A detailed description of each input parameter, as well of the output, is provided in Table 3.2.

4. Graphical user interface demos. Demos for the rrgmres algorithms for symmetric and nonsymmetric linear discrete ill-posed problems (1.1) are included. The demo for problems with a square nonsymmetric matrix is executed with the command `rrgmres_demo`, and the demo for symmetric problems can be run with the command `sym_rrgmres_demo`. Both demos have graphical interfaces that can be used to specify various parameter values. No parameter is required to be input from the command line. Descriptions of the parameters for both demos are presented in Table 4.1. Once the appropriate parameters have been specified, clicking *Run* will execute the demo.

Let $\hat{b}$ denote the unknown error-free right-hand side associated with the error-contaminated right-hand side b of (1.1) and let $\hat{x}$ be the least-squares solution of minimal Euclidean norm of the linear system $Ax = \hat{b}$. Let the iterate x_k satisfy a specified stopping rule. The approximate solution x_k of (1.1) as well as $\hat{x}$ are plotted. The number of iterations, k, the relative error of $\|x_k - \hat{x}\|/\|\hat{x}\|$, as well as the relative residual errors $\|b - Ax_k\|/\|\hat{b}\|$ are displayed for $k = 0, 1, 2, \ldots$.

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TABLE 2.1
Files in rrgmres.zip

File	Description
`baart_alt.m`	Discretization of the Fredholm integral equation of the first kind described by Baart [1] using a Nyström method based on the composite trapezoidal rule with equidistant nodes. The linear discrete ill-posed problem obtained has a square nonsymmetric matrix.
`deriv2_alt.m`	Discretization of a Fredholm integral equation of the first kind that is a Green's function for the second derivative on the interval $[0, 1]$; see, e.g., [2, 5] for a description of the integral equation. The discrete problem is obtained by a Nyström method based on the composite trapezoidal rule with a square matrix. The linear discrete ill-posed problem obtained has a square nonsymmetric matrix. The solution can be chosen to be a discretized linear or exponential function.
`phillips_alt.m`	Discretization of the Fredholm integral equation of the first kind described by Phillips [8] using a Nyström method based on the composite trapezoidal rule with equidistant nodes. The linear discrete ill-posed problem obtained has a square nonsymmetric matrix.
`rrgmres_demo.fig`	The graphical interface for the RRGMRES demo for linear discrete ill-posed problems with a square nonsymmetric matrix.
`rrgmres_demo.m`	The RRGMRES demo for linear discrete ill-posed problem with a square nonsymmetric matrix.
`rrmgres_dp.m`	The RRGMRES algorithm for linear discrete ill-posed problems with a square nonsymmetric matrix. This version uses the discrepancy principle to decide when to terminate the iterations.
`rrgmres_iter.m`	The RRGMRES algorithm for linear discrete ill-posed problems with a square nonsymmetric matrix. This version allows the user to specify the desired number of iterations.
`shaw_alt.m`	Discretization of the Fredholm integral of the first kind discussed by Shaw [9] using a Nyström method based on the composite trapezoidal rule with equidistant nodes. The linear discrete ill-posed problem obtained has a square nonsymmetric matrix.
`sym_rrgmres_demo.fig`	The graphical interface for demo for the RRGMRES method for linear discrete ill-posed problems with a symmetric matrix.
`sym_rrgmres_demo.m`	The demo for the RRGMRES method for linear discrete ill-posed problems with a symmetric matrix.
`sym_rrgmres_dp.m`	The RRGMRES algorithm for linear discrete ill-posed problems with a symmetric matrix. This version uses the discrepancy principle to decide when to terminate the iterations.
`sym_rrgmres_iter.m`	The RRGMRES algorithm for linear discrete ill-posed problems with a symmetric matrix. This version allows the user to specify the number of desired iterations.

REFERENCES

[1] M. L. Baart, The use of auto-correlation for pseudo-rank determination in noisy ill-conditioned least-squares problems, IMA J. Numer. Anal., 2 (1982), pp. 241–247.

[2] L. M. Delves and J. L. Mohamed, Computational Methods for Integral Equations, Cambridge University Press, 1985; p. 310.

[3] P. C. Hansen, Regularization Tools version 4.0 for Matlab 7.3, Numer. Algorithms, 46 (2007), pp. 189–194.

[4] H. W. Engl, M. Hanke, and A. Neubauer, Regularization of Inverse Problems, Kluwer, Dordrecht, 1996.

Table 2.2
Files from Regularization Tools [3]

File	Description
baart.m	Discretization of the Fredholm integral equation of the first kind described by Baart [1] by a Galerkin method with orthonormal piecewise constant test and trial functions. The linear discrete ill-posed problem obtained has a square nonsymmetric matrix.
deriv2.m	Discretization of a Fredholm integral equation of the first kind that is a Green's function for the second derivative on the interval $[0, 1]$; see, e.g., [2, 5] for a description of the integral equation. The discretization is carried out by a Galerkin method with orthonormal piecewise constant test and trial functions. This discretization yields a linear discrete ill-posed problem with a symmetric matrix.
phillips.m	Discretization of the Fredholm integral equation of the first kind described by Phillips [8] by a Galerkin method with orthonormal piecewise constant test and trial functions. This discretization yields a linear discrete ill-posed problem with a symmetric matrix.
shaw.m	Discretization of the Fredholm integral of the first kind discussed by Shaw [9] by a Galerkin method with orthonormal piecewise constant test and trial functions. This discretization yields a linear discrete ill-posed problem with a symmetric matrix.

Table 3.1
Syntax for rrgmres_iter, rrgmres_dp, sym_rrgmres_iter, and sym_rrgmres_iter.

File	Syntax
rrgmres_iter.m	[X,resnrm]=rrgmres_iter(A,b,iterations)
rrgmres_dp.m	[X,resnrm,iterations]= rrgmres_dp(A,b,discrepancy)
sym_rrgmres_iter.m	[X,resnrm]=sym_rrgmres_iter(A,b,iterations)
sym_rrgmres_dp.m	[X,resnrm,iterations]= sym_rrgmres_dp(A,b,discrepancy)

[5] A. K. Louis and P. Maass, A mollifier method for linear operator equations of the first kind, Inverse Problems 6 (1990), pp. 427-440.

[6] A. Neuman, L. Reichel, and H. Sadok, Implementations of range restricted iterative methods for linear discrete ill-posed problems, Linear Algebra Appl., in press.

[7] A. Neuman, L. Reichel, and H. Sadok, Algorithms for range restricted iterative methods for linear discrete ill-posed problems, submitted for publication.

[8] D. L. Phillips, A technique for the numerical solution of certain integral equations of the first kind, J. ACM, 9 (1962), pp. 84–97.

[9] C. B. Shaw, Jr., Improvements of the resolution of an instrument by numerical solution of an integral equation, J. Math. Anal. Appl., 37 (1972), pp. 83–112.

TABLE 3.2

Input parameters for and output from rrgmres_iter, rrgmres_dp, sym_rrgmres_iter, and sym_rrgmres_iter.

Input parameters	**Description**
`A`	The $m \times m$ matrix of the linear discrete ill-posed problem (1.1).
`b`	The right-hand side vector of (1.1).
`iterations`	The number of iterations to carry out. The initial iterate is $x_0 = 0$. The computations are terminated after `iterations` iterations.
`discrepancy`	This stopping criterion allows termination of the iterations based on the discrepancy principle; see [4, 6, 7]. The computations are terminated as soon as an iterate x_k has been determined such that $$\|Ax_k - b\| \leq \texttt{discrepancy}. \quad (3.1)$$ Here x_k denotes the kth iterate; the initial iterate is $x_0 = 0$. The iterations also are terminated when this stopping criterion is not satisfied after m iterations.
Output	**Description**
`X`	An $m \times k$ matrix $X = [x_1, x_2, \ldots, x_k]$, where $x_1, x_2, \ldots, x_k$ are the iterates computed before termination. The initial iterate $x_0 = 0$ is not stored. Thus, k is equal to the input parameter `iterations` when the functions `rrgmres_iter` or `sym_rrgmres_iter` are used. If one applies of the functions `rrgmres_dp` or `sym_rrgmres_dp` instead, then k is the number of iterations carried out before the computations are terminated.
`resnrm`	A vector containing the norm of the residual errors associated with the computed iterates $x_1, x_2, \ldots, x_k$: $$\texttt{resnrm} = [\|Ax_1 - b\|, \|Ax_2 - b\|, \ldots, \|Ax_k - b\|]^T.$$
`iterations`	Output parameter for the functions `rrgmres_dp` and `sym_rrgmres_dp`. This parameter shows the number of iterations that have been carried out when the stopping criterion (3.1) is satisfied. Thus, the value of `iterations` is that of the parameter k above. If `iterations`$= n$, then the value of the last entry of the vector `resnrm` can be used to determine whether or not the stopping criterion (3.1) is satisfied by the last computed iterate.

TABLE 4.1

Description of parameters for `rrmgres_demo` *and* `sym_rrgmres_demo`.

Parameter	Description
Problem section	
Example	A user can choose sample linear discrete ill-posed problems (1.1). For the symmetric demo, the examples use the functions from Table 2.2 that generate linear discrete ill-posed problems with a symmetric matrix. The nonsymmetric demo uses these functions as well as those from Tables 2.1 and 2.2 that generate linear discrete ill-posed problems with a nonsymmetric matrix. The examples require specification of the parameter *Order*, which is the size m in (1.1).
Specified	A user can specify both the matrix and vector.
Error Section	
Seed	Specify a seed for the random number generator.
Relative norm of noise	If the right-hand side b of (1.1) is to be contaminated by an error e, then we let $b = \hat{b} + e$, where $\hat{b}$ is the error-free right-hand side associated with the solution $\hat{x}$, i.e., $A\hat{x} = \hat{b}$. The vector e has normally distributed entries with zero mean. The relative norm of the error in the right-hand side, $\|e\|/\|\hat{b}\|$, can be prescribed.
Iterations Section	
Discrepancy principle	The iterations are terminated when (3.1) holds. We may choose to specify either the value for `discprepancy` or the value for the constant η. By specifying η, with $\eta \geq 1$, `discrepancy` $= \eta\|e\|$ will be calculated. The value for η should be chosen independently of $\|e\|$.
Specified iterations	The algorithm carries out the specified number of iterations. The user-specified number of iterations should be less than m, the order of the problem (1.1) to be solved.