AMS 526 Homework 6, Fall 2018

Due: written part due on Wednesday 12/05 in class;
programming part due on Friday 12/07 by 11:59pm

1. (10 points) In our lectures, it was pointed out that the eigenvalues of a symmetric matrix $A \in \mathbb{R}^{n\times n}$ are the stationary values of the Rayleigh quotient $r(x) = \left(x^T Ax\right) / \left(x^T x\right)$ for $x \in \mathbb{R}^n$. Show that the Ritz values at step k of the Lanczos iteration are the stationary values of $r(x)$ if x is restricted to $\mathcal{K}_k$.

2. (20 points) Suppose $A \in \mathbb{R}^{n\times n}$.

   (a) (5 points) Consider the standard Arnoldi iteration below:

   Algorithm: Arnoldi Iteration

   ```
   given random nonzero b, let q_1 = b/||b||
   for k = 1, 2, 3, ...
       v = A q_k
       for j = 1 to k
           h_jk = q_j^* v
           v = v − h_jk q_j
       h_{k+1,k} = ||v||
       q_{k+1} = v / h_{k+1,k}
   ```

   Determine the number of flops of the Arnoldi iteration at the kth step.

   (b) The standard Arnoldi iteration essentially is based on the modified Gram-Schmidt orthogoalization of the Krylov subspace. We can use Householder transformation. Consider the high-level algorithm below, originally proposed by H.F. Walker (*SIAM J. Sci. Comput.*, 9 (1988)):

   Algorithm: Householder-Arnoldi Iteration

   ```
   given random nonzero b, let v_1 = b
   for k = 1, 2, 3, ...
       compute unit Householder reflector vector w_k such that
           (w_k)_i = 0, i = 1, ..., k − 1, and
           (P_k v_k)_i = 0, i = k + 1, ..., n, where P_k = I − 2 w_k w_k^T
       h_{k−1} = P_k v_k
       q_k = P_1 P_2 ... P_k e_k, where e_k is kth column of the identity matrix
       v_{k+1} ← P_k P_{k−1} ... P_1 A q_k
   ```

   i. (5 points) Give the expression of w_k in terms of v_k.

   ii. (5 points) Determine the number of flops of the Householder-Arnoldi iteration at the kth step. (Note: Pay attention to the efficiency of computing $P_k x$.)

   (c) (5 points) Argue about the potential advantages and disadvantages of the above two iteration strategies.

3. (20 points) Suppose $A \in \mathbb{R}^{n\times n}$ has s distinct eigenvalues.

   (a) (10 points) Suppose that A is diagonalizable. For any $b \in \mathbb{R}^n$, show that the Krylov subspace does not change after at most s iterations.

   (b) (5 points) Suppose A is SPD. Show that the conjugate gradient method arrives at the exact solution of $Ax = b$ in at most s iterations under exact arithmetic.

(c) (5 points) Suppose A is symmetric. Generalize the argument for part (b) to the method of MINimal RESidual (MINRES).

4. (20 points) Given $A \in \mathbb{R}^{n\times n}$, the CGN is a method that applies CG to the normal equation $A^T Ax = A^T b$. GMRES is a method that finds the minimum norm solution at each step within the Krylov subspace.

   (a) Suppose A is a unitary matrix. Show that CGN converges in one step.

   (b) Consider the circulate matrix of the form

$$A = \begin{bmatrix} 0 & 1 & & & \\ & 0 & 1 & & \\ & & \ddots & \ddots & \\ & & & 0 & 1 \\ 1 & & & & 0 \end{bmatrix}.$$

   Show that it is a unitary matrix with n distinct eigenvalues, and hence GMRES may require up to n steps to converge.

5. (30 points) Implement the conjugate gradient method and the preconditioned conjugate gradient method with the Jacobi preconditioner for solving SPD linear systems. (Note: Do not use MATLAB's builtin implementation of pcg for this assignment.) Apply the methods to the following model problem:
   Suppose the unknowns are given as a two dimensional array x_{ij}, where $i, j = 0, \dots, n+1$. Let $h = 1/(n+1)$, and each equation in the system satisfies

$$(4 + h^2)x_{i,j} - x_{i-1,j} - x_{i+1,j} - x_{i,j-1} - x_{i,j+1} = h^2,$$

   for $i, j = 1, \dots, n+1$, and $x_{0,j} = x_{n+1,j} = x_{i,0} = x_{i,n+1} = 0$. The system represents a finite difference approximation of the boundary value problem $-\Delta u + u = 1$ in $\Omega = (0,1)\times(0,1)$ and $u = 0$ on the boundary of Ω.
   Take $n = 8, 16, 32$. Compare their performance in terms of rate of convergence.