Scientific Computing, Spring 2002 (http://www.math.nyu.edu/faculty/goodman/teaching/SciComp2002/)

Assignment 4.

Given February 21, due February 28.

Objective: Numerical Linear Algebra

1. Verify the formula for the sum of a geometric series:

$$1 + x + x^{2} + \dots + x^{n-1} = \begin{cases} \frac{1-x^{n}}{1-x} & , & \text{if } x \neq 1. \\ n & , & \text{if } n = 1. \end{cases}$$
(1)

Meant to be a very quick paper and pencil exercise.

2. The "discrete Fourier transform", or DFT, is an $n \times n$ matrix, Q, whose entries are given by

$$q_{jk} = \frac{1}{\sqrt{n}} z^{(j-1)(k-1)}$$
, where $z = e^{2\pi i/n}$. (2)

The number z is a "primative n^{th} root of unity, meaning that $z^n = 1$ but $z^m \neq 1$ when $1 \leq k < n$. Remember that for any integer $p, z^{pn} = (z^n)^p = 1^p = 1$. To show that Q is a unitary matrix, we need to compute the entries of Q^*Q . Show that the (j, k) entry of Q^*Q is

$$\sum_{l=1}^{n} \overline{q}_{lj} q_{lk}$$

interpret this as a constant times a geometric series, and determine the sum. Show from this that the entries of Q^*Q are what they must be when Q is unitary. We will see that the DFT has many applications in scientific computing. *Meant to be a somewhat* more challenging paper and pencil exercise to introduce the DFT.

3. Download the matlab script eigtest.m and examine it. Check that the computed eigenvalues of A are real and that Q is actually unitary. For small n = 5, check that the computed eigenvalues of A and $B = Q^*AQ$ are nearly equal. Since the eigenvalues of A a are real, if the computed eigenvalues of B have an imaginary part, this must be due to roundoff and possible error amplification through ill conditioning. Run the script for n values ranging up to 140 or as high as your computer can easily go and examine the plots, in view of the theory of eigenvalue conditioning for the nonsymmetric eigenvalue problem. Do the imaginary parts of the computed eigenvalues of B depend on the condition number as the theory suggests they should? You might want to pretty up the code. In particular, create labels for the axes in the plots and write titles on the plots. Hopefully very easy computer exercise that leads you to think through and comment on the material on the condition number of the eigenvalue problem.

4. Write a procedure in C/C++ to compute the Choleski decomposition of a positive definite symmetric matrix. Your procedure should take an $n \times n$ real symmetric matrix, A, and compute an $n \times n$ lower triangular matrix, L, with $LL^* = A$. It might be convenient to store only the lower triangular entries (including the diagonal) or it might be easier to store the whole matrix but assume that $a_{jk} = a_{kj}$. There are n square roots to take in this process. Your procedure should return an error flag if any of these is not real. Make sure also to write a procedure that computes LL^* from a lower triangular matrix L to check that your factor is correct. Apply your Choleski factorization procedure to the $n \times n$ matrix

$$A(s) = \begin{pmatrix} 2 & 1 & 1 & \cdots & 1 \\ 1 & 2 & 1 & 1 & \cdots & 1 \\ 1 & 1 & 2 & 1 & \cdots & 1 \\ \vdots & & \ddots & & \vdots \\ 1 & \cdots & & 1 & 2 \end{pmatrix} - s \begin{pmatrix} 2 & 1 & 0 & \cdots & 0 \\ 1 & 2 & 1 & 0 & \cdots & 0 \\ 0 & 1 & 2 & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & & 1 & 2 \end{pmatrix}$$

Write a procedure to apply forward and back substitution on given Choleski factors and a tester to make sure the answer is correct. Use your Choleski and back substitution procedures to make a plot of $x_1(s)$ (the first component of x(s) where $A(s)x(s) = e_1$ (the "standard" basis vector with one in the first entry and the rest zero). Starting from s = 0 and stopping at the first place where A(s) is determined not to be positive definite. In your program, this means that we attempt to compute the Choleski factor of A(s) and continue until the Choleski factorization procedure returns an error flag indicating that this is impossible. Take steps $\Delta s = .01$ and n = 20. This involves considerable programming. Make sure to hand in both procedures and both testers, runs indicating the tests work, as well as the graphs requested. We will use this Choleski code in later assignments.