YALE UNIVERSITY DEPARTMENT OF COMPUTER SCIENCE

CptSci 440/540: Numerical Computation I $\begin{array}{c} \textit{Handout} \ \# \\ \textit{January 23, 2015} \end{array}$

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Problem Set 1

Due Date: February 13

Write a code that uses the double Gram-Schmidt procedure to invert a given square matrix A. Use the fact that

$$A \cdot G = U \quad \Rightarrow \quad A^{-1} = I \cdot G \cdot U^*,$$

where I is the identity matrix, U is an orthogonal matrix and U^* is the adjoint (transpose) of U. That is, one may obtain the matrix G by applying the same set of transformations to I as is applied to A in the Gram-Schmidt procedure.

In Fortran, your calling sequence should be

$$inv_double_gs(a, n, u, b)$$
 (1)

where

a(n,n) is a (real*8) $n \times n$ -matrix to be inverted (input parameter)

n is the (integer) size of the matrix (input parameter)

u(n,n) is a (real*8) $n \times n$ -matrix (output parameter). The matrix u is orthogonal, and its columns are the result of the double Gram Schmidt process applied to the columns of a

b(n,n) is a (real*8) $n \times n$ -matrix (output parameter). The matrix b is the inverse of a

In C, your calling sequence should be

$$void\ inv_double_qs(double*\ a, int\ n, double*\ u, double*\ b),$$
 (2)

where

a points to an array of doubles of size n^2 , containing $a(1,1), a(1,2), \ldots, a(1,n), a(2,1), \ldots, a(n,n)$, a being the $n \times n$ matrix to be inverted (input parameter)

n is the (integer) size of the matrix (input parameter)

u points to an array of doubles of size n^2 , containing $u(1,1), u(1,2), \ldots, u(1,n), u(2,1), \ldots, u(n,n)$, u being the $n \times n$ orthogonal matrix. The columns of u are the result of the double Gram-Schmidt process applied to the columns of u (output parameter, memory allocated by the user)

b points to an array of doubles of size n^2 , containing $b(1,1), b(1,2), \ldots, b(1,n), b(2,1), \ldots, b(n,n)$, being the $n \times n$ matrix. The matrix b is the inverse of a (output parameter, memory allocated by the user)

REMARK 1. Make sure that the calling sequence of your function is exactly as specified in the assignment.

REMARK 2. Test your code before submission. In particular, make sure that the matrix u is indeed orthogonal and b is indeed the inverse of a.