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AMS 213: Numerical Solutions
Project 1: Midterm
QR vs. Cholesky for Best Fit Polynomials
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Question 1 : QR Decomposition Routine

The custom subroutine below, called QRDECOMP, takes a non-square nxm matrix A and returns the QR decomposition of A as two matrices, Q and R.

SUBROUTINE QRDECOMP(a,q,r)
Parameters :: a(input) nxm matrix, q(output), r(output)
Returns QR decomposition of a non-square nxm matrix

Question 2 : QR Backsubstitution

This subroutine uses the upper diagonal matrix R to solve a linear system of equations using backsubstitution. First, right hand side is multiplied by Q^T and then the system is solved using backsubstitution. As inputs, the routine takes two matrices: A and b, where b is a RHS vector of size mx1 and where A is an mxm matrix. The solution is returned in matrix b.

SUBROUTINE QRSOLVE(a,b)
Solves A x = B using Q R x = b → R x = Q^T b
Parameters :: Input: nxn matrix A and nx1 matrix B, Output: Solution in matrix B
Returns solution in matrix B
Uses QRDECOMP subroutine for QR decomposition of A

Question 3 : Comparison of QR and Cholesky with Atkinson data

This subroutine reads data file with two columns of x,y coordinates and produces an n-order polynomial least square fit using QR method. Returns data file containing the parameters of the fit and the RMS error of the fit. Also returns a data file containing x,y coordinates of the fitted data.

SUBROUTINE QRLEASTSQUARES(order,parameters,filename,filename2,filename3)

Parameters ::

Inputs: integer order (order of polynomial to fit dataset),
character filename,filename2,filename3
Outputs: real,dimension(:) :: parameters (unallocated vector to store result parameters)
character filename2 (output parameter file),filename3 (output fit data coordinates)

usage: call QRLEASTSQUARES(3,parameters,'atkinson.dat','qrparameters.dat','qrfit.dat')

Question 4 : Failure of Cholesky Method

This modified cholesky fit routine is based on a routine constructed from Homework #3 but is modified to include an input parameter to set the order of the fit polynomial

This subroutine reads data file with two columns of x,y coordinates and produces an n-order polynomial least square fit using the cholesky method. It returns a data file containing the parameters of the fit and the RMS error of the fit. Also returns a data file containing x,y coordinates of the fitted data.

SUBROUTINE CHOLESKYLEASTSQUARES(order,parameters,filename,filename2,filename3)

Parameters ::

Inputs: integer order (order of polynomial to fit dataset),
character filename,filename2,filename3
Outputs: real,dimension(:) :: parameters (unallocated vector to store result parameters)
character filename2 (output parameter file),filename3 (output fit data coordinates)

usage: call CHOLESKYLEASTSQUARES(3,parameters,'atkinson.dat','choleskyparameters.dat','choleskyfit.dat')

The performance of the Cholesky and QR best fit routines was compared with the atkinson data with varying fit polynomial order. The RMS error of each is shown below in Figure 1. The cholesky algorithm returned NaN (invalid numbers) in line fits with polynomials of order 7 and greater.

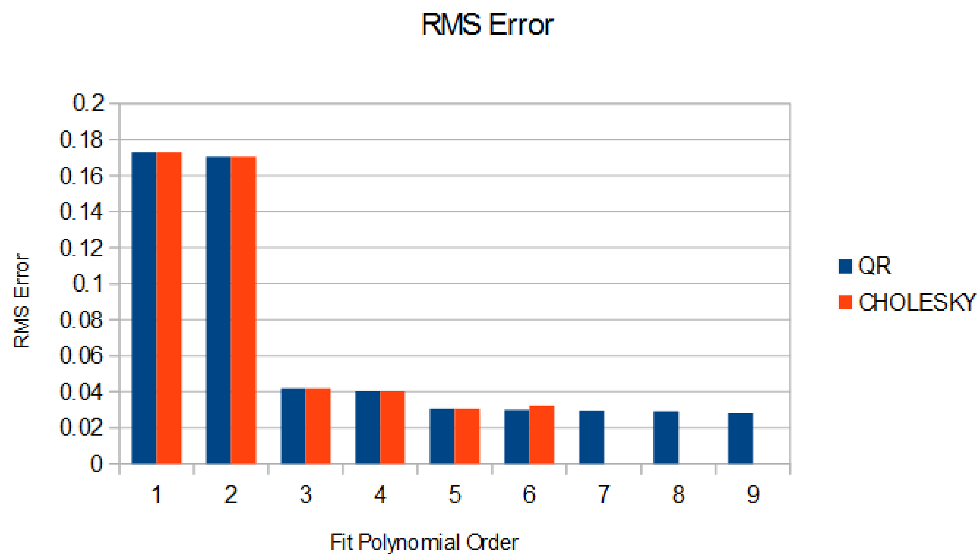

Figure 1: RMS Error of QR and Cholesky best fit polynomials

Question 5 : What is happening?

The condition number of a function is a measure of the worst-case relative change in output for a change in input. For example, a measure of how small errors in the input of a function affect the output of the function. With a system of matrices, $Ax = b$, the condition number is roughly the rate at which the solution, x, changes with respect to the input, b. If the condition number is infinite, the algorithm will not reliably find a solution to the problem.

Condition number is defined as the product of the norm of A and the norm of A-inverse.

$$\varepsilon = ||A||\ ||A^{-1}||$$

It follows that if matrix A has condition number ε, then the condition number of $A^T A$ is $\varepsilon^* = ||A^T A||\ ||(A^T A)^{-1}|| = ||A||^2\ ||A^{-1}||^2$, which is clearly larger than the condition number of A .

Vandermonde matrices are used to create the matrix A in the linear system $Ax = b$ using (x,y) coordinate data in order to calculate best-fit polynomials. The condition number of the vandermonde matrix created may be very large.

For numerical solutions is it desirable to compute an orthonormal basis for a space since errors are not magnified when multiplying with an orthogonal matrix. The QR method uses orthogonal Householder matrices which have a condition number of 1.

In solving $Ax = b$ with the Cholesky method, we have $A^T A\, x = A^T b$ so we must first compute $A^T A$ and $A^T b$. In computing $A^T A$, for the reason presented above, the condition number is increased. Because of the poor stability properties of the Cholesky method, it is rarely used for least-square problems.

This implies that the condition number of both QR and Cholesky least square approaches should be equal for input data where the number of data points is equal to the order of the polynomial, which results in a square matrix A.

References

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