Lab Session 5

MA-423 :   Matrix Computations   July - November 2019   S. Bora

1. Write a MATLAB function program $[\mathtt{Q}, \mathtt{R}] = \mathtt{cgs(V)}$ to orthonormalize the columns of an $n \times m$ matrix V, $(n \geq m)$ by the Classical Gram Schmidt procedure so that Q is the isometry satisfying

$$
\begin{aligned}
\operatorname{span}\{Q(:,1)\} &= \operatorname{span}\{V(:,1)\} \\
\operatorname{span}\{Q(:,1), Q(:,2)\} &= \operatorname{span}\{V(:,1), V(:,2)\}, \\
&\vdots \\
\operatorname{span}\{Q(:,1), Q(:,2), \ldots, Q(:,m)\} &= \operatorname{span}\{V(:,1), V(:,2), \ldots, V(:,m)\}
\end{aligned}
$$

   and R is an upper triangular matrix such that $R(i,j) = \langle V(:,j), Q(:,i) \rangle$.

2. A slight modification of the above program leads to the Modified Gram Schmidt procedure for orthonormalizing the columns of V. Perform this modification to obtain another function program $[\mathtt{Q}, \mathtt{R}] = \mathtt{mgs(V)}$.

3. Write a function program $[\mathtt{Q}, \mathtt{R}] = \mathtt{cgsrep(V)}$ that performs Classified Gram Schmidt with reorthogonalization by making appropriate changes to your function program $\mathtt{cgs}$.

   Take care to replace *for loops* by matrix-vector multiplications as far as possible in each of the above programs.

4. The purpose of this exercise is to solve the Least-Squares Problem (in short, LSP) $Ax = b$ by different methods and compare the solutions. Here $A \in \mathbb{R}^{n \times m}$ and $b \in \mathbb{R}^n$, and usually n is much bigger than m.

   Origin: Suppose that we have a data set (t_i, b_i), for $i = 1 : m$, that have been obtained from some experiment. These data are governed by some unknown laws. So, the task is to come up with a model that best fits these data. A model is generated by a few functions, called model functions, $\phi_1, \ldots, \phi_n$. Therefore once a model is chosen, the task is to find a function p from the span of the model functions that best fits the data.

   Suppose that the model functions $\phi_1, \ldots, \phi_n$ are given. For $p \in \operatorname{span}(\phi_1, \ldots, \phi_n)$, we have $p = x_1 \phi_1 + \cdots + x_n \phi_n$ for some $x_j \in \mathbb{R}$. Now, forcing p to pass through the data (t_i, b_i) for $i = 1 : m$, we have $p(t_i) = b_i + r_i$, where r_i is the error. We want to choose that p for which the sum of the squares of the errors r_i is the smallest, that is, $\sum_{i=1}^{m} |r_i|^2$ is minimized.

   Now $p(t_i) = b_i + r_i$ gives $x_1 \phi_1(t_i) + \cdots + x_n \phi_n(t_i) = b_i + r_i$. Thus in matrix notation,

$$
\begin{bmatrix} \phi_1(t_1) & \cdots & \phi_n(t_1) \\ \phi_1(t_2) & \cdots & \phi_n(t_2) \\ \vdots & \cdots & \vdots \\ \phi_1(t_m) & \cdots & \phi_n(t_m) \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{bmatrix} + \begin{bmatrix} r_1 \\ r_2 \\ \vdots \\ r_m \end{bmatrix}.
$$

   This is of the form $Ax = b + r$ and we have to choose $x \in \mathbb{R}^n$ for which the 2-norm of the residual vector $\|r\|_2$, is minimized. We write this as LSP $Ax = b$.

Your task is to find the polynomial of degree 19 that best fits the function $f(t) = \sin(\frac{\pi}{5}t) + \frac{t}{5}$ for $t_1 = -5, t_2 = -4.5, \ldots, t_{23} = 6$. Set up the LSP $Ax = b$ and determine the polynomial p whose coefficients are determined by x in three different ways:

(a) By using the Matlab command
>> A \ b
This uses QR factorization to solve the LSP $Ax = b$. Call this polynomial p_1.

(b) By setting up the normal equation $A^T Ax = A^T b$ and solving them for x. You will need to use the Cholesky method for this. Call this polynomial p_2.

(c) By solving the argumented system $\begin{bmatrix} I_n & A \\ A^T & 0 \end{bmatrix} \begin{bmatrix} -r \\ x \end{bmatrix} = \begin{bmatrix} b \\ 0 \end{bmatrix}$. Call this polynomial p_3.

Set the formatting to `format long e` and compute the condition number of the coefficient matrix associated with each of the systems that you are solving. Which one is the most ill conditioned?

Compute the $\|r\|_2$ which gives the value of $\sqrt{\Sigma_{i=1}^{23}|p_j(t_i) - f(t_i)|^2}$ $j = 1, 2, 3$ for each of these methods (again in `format long e.`). This is a measure of the goodness of the fit in each case. Which of the methods provide the best fit?