EECE 7220 / 8220: Scientific Computing

Fall 2018

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Homework: 5

Due: Dec 11, 2018 by 12.30 pm (noon)

Submission Instructions:

- Upload your programs to the homework dropbox in http://elearn.memphis.edu.
  - There should be a main program that we can run to automatically generate results, and plots for all the problems. We run your programs for grading your homework solutions. So, make sure that we can run your programs from a main program.
- Prepare a PDF report of your solution / results (solution vector, etc.) and any inferences for the problems and upload the PDF report to the homework dropbox.
  - Do not include/copy-paste programs in your report.

Grade Distribution:

- Structured and complete report: 5 points
- Implementation of GMRES: 45 points
- 2a: 15 points
- 2b: 10 points
- 2c: 10 points
- 3a: 5 points
- 3b: 5 points

Learning Objective: To understand generalized minimum residual (GMRES)–a Krylov subspace approach to solve $A\vec{x} = \vec{b}$

Data Generation: To evaluate GMRES (programs), generate test data $\{(x_i, y_i)\}_{i=1}^{11}$ that has a decic relationship as follows:

1. Let the underlying relationship between variables x_i (independent) and y_i (dependent) be decic (10th order polynomial). i.e. $y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \cdots + \beta_{10} x_i^{10}$.

2. Let, $\vec{\beta} = \begin{bmatrix} 1 \\ -567/1562500 \\ 64161/6250000 \\ -11727/100000 \\ 4523/6250 \\ -10773/4000 \\ 63273/10000 \\ -189/20 \\ 8.7 \\ -4.5 \\ 1 \end{bmatrix}$; $\vec{x} = \begin{bmatrix} -0.9000 \\ -0.7200 \\ -0.5400 \\ -0.3600 \\ -0.1800 \\ 0 \\ 0.1800 \\ 0.3600 \\ 0.5400 \\ 0.7200 \\ 0.9000 \end{bmatrix}$

3. Generate 11 data points $\{(x_i, y_i)\}_{i=1}^{11}$ from the decic model:
   $y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \cdots + \beta_{10} x_i^{10}$

4. Now the generated data points $\{(x_i, y_i)\}_{i=1}^{11}$ lie exactly on a decic polynomial.

5. To estimate the decic model parameters $\vec{\beta}$ from the generated data points $\{(x_i, y_i)\}_{i=1}^{11}$, we need to solve: $X_{11\times 11}\vec{\beta}_{11\times 1} = \vec{y}_{11\times 1}$

AUXILIARY ALGORITHMS

Generalized Minimum Residual (GMRES):

Input :

1. A: system matrix
2. $\vec{b}$: right-side vector
3. $\vec{x}_0$: an initial guess for the unknown $\vec{x}$
4. k: number of Krylov subspaces to find the unknown $\vec{x}$

Output: $\vec{x}$

$\vec{r}_0 \leftarrow \vec{b} - A\vec{x}_0$;
$\vec{v}_1 \leftarrow \vec{r}_0 / \|\vec{r}_0\|$;
for $i \leftarrow 1, 2, \ldots, k$ **do**
    $\vec{w}_i \leftarrow A\vec{v}_i$;
    for $j \leftarrow 1, 2, \ldots, i$ **do**
        $h_{j,i} \leftarrow (\vec{w}_i, \vec{v}_j)$;
        $\vec{w}_i \leftarrow \vec{w}_i - h_{j,i}\vec{v}_j$;
    end
    $h_{i+1,i} \leftarrow \|\vec{w}_i\|$;
    $\vec{v}_{i+1} \leftarrow \vec{w}_i / h_{i+1,i}$;
    Find $\vec{y}_i \in \mathbb{R}^i$ which minimizes the current residual $\|\vec{r}_i\| \leftarrow \| \|\vec{r}_0\| \vec{e}_i - \tilde{H}_i \vec{y} \|$;
    <u>Note 1</u>: Solve the above optimization problem using your previous QR decomposition and back-substitution procedure (refer to your Homework 04, problem 1 solution) ;
    <u>Note 2</u>: Hessenberg matrix $\tilde{H}_i = \begin{bmatrix} h_{p,q} \end{bmatrix} \in \mathbb{R}^{(i+1)\times i}$; and $\vec{e}_i = \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \in \mathbb{R}^{i+1}$;
    if $\|\vec{r}_i\| < \epsilon$ **then**
        $\vec{x}_i \leftarrow \vec{x}_0 + \begin{bmatrix} \vec{v}_1, \ldots, \vec{v}_i \end{bmatrix} \vec{y}_i$;
        Stop ;
    end
end

Algorithm 1: Generalized Minimum Residual (GMRES) Procedure

Modified Gram-Schmidt Orthogonalization Procedure:

Input : A set of r linearly independent vectors $\{\vec{x}_1, \vec{x}_2, \ldots, \vec{x}_r\}$

Output: A set of r orthonormal vectors $\{\vec{q}_1, \vec{q}_2, \ldots, \vec{q}_r\}$ such that
$\texttt{Span}\left(\{\vec{x}_i\}_{i=1}^r\right) = \texttt{Span}\left(\{\vec{q}_i\}_{i=1}^r\right)$

$r_{11} \leftarrow \|\vec{x}_1\|$;
if $r_{11} = 0$ **then**
  Stop
else
  $\vec{q}_1 \leftarrow \frac{x_1}{r_{11}}$
end
for $j \leftarrow 2$ **to** r **do**
  $\hat{q} \leftarrow \vec{x}_j$;
  for $i \leftarrow 1$ **to** $j-1$ **do**
    $r_{ij} = (\hat{q}, \vec{q}_i)$;
    $\hat{q} = \hat{q} - r_{ij}\vec{q}_i$;
  end
  $r_{jj} \leftarrow \|\hat{q}\|$;
  if $r_{jj} = 0$ **then**
    Stop;
  else
    $\vec{q}_j = \frac{\hat{q}}{r_{jj}}$;
  end
end

Algorithm 2: Modified Gram-Schmidt Orthogonalization Procedure

Back-substitution Procedure *to solve* $R\vec{\beta} = \vec{y}$:

Input : 1. An upper triangular matrix $R \in \mathbb{C}^{n\times n}$; and 2. right-side vector $\vec{y} \in \mathbb{C}^{n\times 1}$

Output: $\vec{\beta} \in \mathbb{C}^{n\times 1}$

for $j \leftarrow n$ **to** 1 **do**

$$\beta_j = \frac{y_j - \sum_{k=j+1}^{n} \beta_k \, r_{jk}}{r_{jj}}$$

end

Algorithm 3: Back-substitution procedure

Homework Problem:

1. Write a program to implement the GMRES algorithm given above.
2. Using the data generated above, solve $X_{11\times 11}\vec{\beta}_{11\times 1} = \vec{y}_{11\times 1}$ for $\vec{\beta}_{11\times 1}$ using the GMRES algorithm. For your GMRES program, use an initial guess for the solution as $\vec{\beta}_0 = \vec{0}$ and $k = 11$.
   (a) Write your observations specifically about how GMRES is converging (i.e. how $\|\vec{r}_i\|$ in line 14 of the GMRES algorithm changes with the Arnoldi iteration i – the "For" loop between lines 3 and 18).
   (b) Observe what happens when $k = 5$ and $k = 3$. How is the convergence affected ? How does your estimate of the unknown $\vec{\beta}$ compare to the true value of $\vec{\beta}$ chosen for data generation ?
   (c) What do the choices of $k = 11, 5, 3$ in the GMRES algorithm imply ? (Hint: Solution in the sequence of Krylov subspaces).
3. **Plots**:
   (a) Plot the magnitude of the residual error $\|\vec{r}_i\|$ vs Arnoldi iteration number i for $k = 3, 5, 11$
   (b) Compare the scatter plot of the actual data that you generated $\{x_i, y_i\}_{i=1}^{11}$ and compare to the scatter plot of the estimated responses $\{x_i, \hat{y}_i\}_{i=1}^{11}$. Where, $\hat{y}_i = \beta_0 + \beta_1 x_i + \cdots + \beta_{10} x_i^{10}$ with $\vec{\beta}$ estimated using GMRES.