Norwegian University of Science and Technology
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TMA4205 Numerical Linear Algebra Fall 2017

Exercise set 3

1 (Cf. Exercise 6.8 in Saad.) Consider the solution of the linear system $Ax = b$ with initial guess x_0, where

$$A = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}, \qquad b = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \qquad x_0 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}.$$

a) Compute the matrices V_m and H_m, $m = 1, \ldots, 5$, resulting from the application of Arnoldi process.

b) Compute the FOM iterates y_m, x_m, $m = 1, \ldots, m$ (when possible).

c) Describe in detail the QR factorization of the matrices $\tilde{H}_m$, $m = 1, \ldots, 5$, using Givens rotations.

d) Compute the GMRES iterates y_m, x_m, $m = 1, \ldots, m$ (when possible).

Possible solution

a) Given the data, the "naive" basis for the Krylov subspace is orthonormal; in fact it is the canonical basis in $\mathbb{R}$'5: $A^k r_0 = A^k b = A^k e_1 = e_{k+1}$, $k = 0, \ldots, 4$. Therefore $V_m = [e_1, \ldots, e_m]$ after m steps of the Arnoldi process. A direct computation shows that

$$\tilde{H}_5 = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

from which the submatrices $\tilde{H}_k$, $k = 1, \ldots, 4$, can be deduced. Note that $h_{6,5} = 0$, that is, the Arnoldi process (understandably) "breaks down" at this iteration, as $\mathcal{K}_5(A, r_0)$ spans the whole space.

b) At iteration 1 we need to find a Givens rotation that "eliminates" the second component of the vector $(0, 1)^T$. Using e.g. formulas at the top of p. 168 in [Saad], we find

$$\Omega_1 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \qquad \text{and} \qquad \tilde{R}_1 = \Omega_1 \tilde{H}_1 = \Omega_1 \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

The same holds at iterations $k = 2, 3, 4$ with $\Omega_k = \Omega_1$ and $R_k = \mathrm{Id}_k$. The matrix $\tilde{R}_5$ can be computed from the QR-factorization of $\tilde{H}_4$ as follows: First, we compute

$$\begin{pmatrix} Q_4 & 0 \\ 0 & 1 \end{pmatrix} \tilde{H}_5 = \begin{pmatrix} Q_4 \tilde{H}_4 & Q_4 e_1 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} \tilde{R}_4 & e_5 \\ 0 & 0 \end{pmatrix},$$

where Q_4 is the result of successive application of $\Omega_1, \ldots, \Omega_4$ to rows $(1, 2), \ldots, (4, 5)$, e_i is the i-th canonical basis vector in $\mathbb{R}^5$, and we used the easily verifiable formula $Q_k e_1 = (-1)^k e_{k+1}$, $k = 1, \ldots, 4$. Since the resulting matrix is already upper triangular, we can simply take $\Omega_5 = \mathrm{Id}_2$, the 2×2 identity matrix. In particular, $R_5 = \mathrm{Id}_5$.

c) To solve the least squares problems appearing in GMRES we need to find $\bar{g}_k = Q_k(\beta e_1)$, where $\beta = \|r_0\|_2 = 1$. For $k = 1, \ldots, 4$ we get $\bar{g}_k = (-1)^k e_{k+1}$, and for $k = 5$ we get $\bar{g}_5 ? e_5 \in \mathbb{R}^6$. Knowing that $R_k = \mathrm{Id}_k$, $k = 1, \ldots, 5$ we compute $y_k = R_k^{-1} \bar{g}_k$, which results in $y_k = 0$, $k = 1, \ldots, 4$, and $y_5 = e_5$. Finally we get $x_k = x_0 + V_k y_k$, resulting in $x_k = x_0$, $k = 1, \ldots, 4$, and $x_5 = e_5$.

2 Assume that $A \in \mathbb{R}^{n \times n}$ is SPD and that we use the CG method for solving the system $Ax = b$. Assume moreover that the eigenvalues $\lambda_1, \ldots, \lambda_{n-1}$ are distributed in an interval $[\lambda_{\min}, \lambda_{\max}] \subset \mathbb{R}_{>0}$, while the eigenvalue λ_n is "very different" from the others (that is, either much larger than $\lambda_{\max}$ or much closer than $\lambda_{\min}$ to 0).

Find an estimate for the error reduction $\|x_m - x^*\|_A / \|x_0 - x^*\|_A$ after m steps of the CG method. Here $x^* = A^{-1} b$ is the exact solution of the system. The estimate should only depend on $\lambda_{\max}$, $\lambda_{\min}$, λ_n, and m.

Possible solution

We use the estimate (cf. the second equation in the proof of Saad, Theorem 6.29)

$$\frac{\|x_m - x^*\|_A}{\|x_0 - x^*\|_A} \leq \max_{i=1,\ldots,n} |r(\lambda_i)|$$

for every polynomial r of degree at most m with $r(0) = 1$.

Moreover, we know from Saad, Theorem 6.25, that with

$$p(\lambda) = \frac{C_{m-1}\Big(1 + 2\frac{\lambda - \lambda_{\max}}{\lambda_{\max} - \lambda_{\min}}\Big)}{C_{m-1}\Big(1 - 2\frac{\lambda_{\max}}{\lambda_{\max} - \lambda_{\min}}\Big)},$$

where C_{m-1} denotes the Chebyshev polynomial, we have $p(0) = 1$ and

$$\max_{\lambda \in [\lambda_{\min}, \lambda_{\max}]} |p(\lambda)| = \frac{1}{C_{m-1}\Big(1 - 2\frac{\lambda_{\max}}{\lambda_{\max} - \lambda_{\min}}\Big)}.$$

Following the computations after the proof of Saad, Theorem 6.29, we can estimate this further by

$$\max_{\lambda \in [\lambda_{\min}, \lambda_{\max}]} |p(\lambda)| \leq 2\left(\frac{\sqrt{\lambda_{\max}} - \sqrt{\lambda_{\min}}}{\sqrt{\lambda_{\max}} + \sqrt{\lambda_{\min}}}\right)^{m-1}.$$

Now define

$$r(\lambda) = p(\lambda)\frac{\lambda_n - \lambda}{\lambda_n}.$$

Then $r(0) = 1$ and $r(\lambda_n) = 0$. Thus

$$\begin{aligned}
\max_{i=1,\dots,n} |r(\lambda_i)| &\le \max_{i=1,\dots,n-1} |p(\lambda_i)| \frac{|\lambda_n - \lambda_i|}{\lambda_n} \\
&\le \max_{\lambda \in [\lambda_{\min}, \lambda_{\max}]} |p(\lambda)| \frac{|\lambda_n - \lambda|}{\lambda_n} \\
&\le 2\left(\frac{\sqrt{\lambda_{\max}} - \sqrt{\lambda_{\min}}}{\sqrt{\lambda_{\max}} + \sqrt{\lambda_{\min}}}\right)^{m-1} \max_{\lambda \in [\lambda_{\min}, \lambda_{\max}]} \frac{|\lambda_n - \lambda|}{\lambda_n}.
\end{aligned}$$

Thus, if $\lambda_n > \lambda_{\max}$, we have

$$\frac{\|x_m - x^*\|_A}{\|x_0 - x^*\|_A} \le 2\left(\frac{\sqrt{\lambda_{\max}} - \sqrt{\lambda_{\min}}}{\sqrt{\lambda_{\max}} + \sqrt{\lambda_{\min}}}\right)^{m-1} \left(1 - \frac{\lambda_{\min}}{\lambda_n}\right),$$

whereas for $\lambda_n < \lambda_{\min}$ we have

$$\frac{\|x_m - x^*\|_A}{\|x_0 - x^*\|_A} \le 2\left(\frac{\sqrt{\lambda_{\max}} - \sqrt{\lambda_{\min}}}{\sqrt{\lambda_{\max}} + \sqrt{\lambda_{\min}}}\right)^{m-1} \left(\frac{\lambda_{\max}}{\lambda_n} - 1\right).$$

3 (Cf. Problem 3a, exam 2016.) We are given a linear system of the form

$$(I + uu^T)x = b,$$

where $I \in \mathbb{R}^{n \times n}$ is the n-dimensional identity matrix and $u \in \mathbb{R}^{n \setminus \{0\}}$ is some given non-zero vector. Assume we apply the CG-method for solving this system. How many iterations do you expect the method to take until convergence is reached?

Possible solution

The matrix uu^T is of rank one and has the unique non-zero eigenvalue $\|u\|_2^2$ with eigenvector u (as $uu^T u = \|u\|_2^2 u$). Thus the matrix $I + uu^T$ has the eigenvalues 1 and $1 + \|u\|_2^2$. Since there are only two distinct eigenvalues, it follows that the CG-method will converge after at most two steps.