SF3580

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1 Task 2

1.1 (a)

Insert figure

1.2 (b)

Insert figure

1.3 (c)

Insert figure

The Rayleigh quotient only uses the symmetric part of A in

$$r(\mathbf{x}) = \mathbf{x}^H A\mathbf{x}$$

assuming $\mathbf{x}$ is normalized. The matrix A is no longer symmetric, i.e. $A \neq A^H$, but any square matrix can be decomposed into a symmetric part A_s and a nonsymmetric part A_{ns} by

$$A = \underbrace{\frac{1}{2}\left(A + A^H\right)}_{=A_s} + \underbrace{\frac{1}{2}\left(A - A^H\right)}_{=A_{ns}}.$$

Thus

$$r(\mathbf{x}) = \mathbf{x}^H A_s\mathbf{x} + \mathbf{x}^H A_{ns}\mathbf{x} = \mathbf{x}^H A_s\mathbf{x}$$

since

$$\mathbf{x}^H A_{ns}\mathbf{x} = \mathbf{x}^H A\mathbf{x} - \mathbf{x}^H A^H\mathbf{x} = 0.$$

For a nonsymmetric matrix all avaliable information is not used.

2 Task 3

The performance of different versions of Gram-Schmidt orthogonalisations is investigated when combined with the Arnoldi method. We consider the matrix A constructed by

```
Random.seed!(0); A=matrixdepot("wathen",nn,nn)
```
(1)

where we choose $nn = 500$ and use m number of iterations in the Arnoldi method. Results for CPU time and orthogonality of the basis in Q is given in Table 1. It can be concluded that double Gram-Schmidt performs the best in terms of orthogonalization error, while single Gram-Schmidt is the fastest among

Table 1: Comparison for different types of Gram-Schmidt (GS) orthogonalisation in the Arnoldi method: SGS (single GS), MDS (modified GS), DGS (double GS), TGS (triple GS), where *time* is the measured CPU time and *orth* is the orthogonality of the basis in terms of $\|Q_m^T Q_m - I\|$.

m	SGS time	SGS orth	MGS time	MGS orth	DGS time	DGS orth	TGS time	TGS orth
5	188 ms	$4.82 \cdot 10^{-13}$	241 ms	$3.28 \cdot 10^{-15}$	246 ms	$3.81 \cdot 10^{-15}$	298 ms	$3.84 \cdot 10^{-15}$
10	496 ms	$2.15 \cdot 10^{-12}$	705 ms	$1.32 \cdot 10^{-14}$	665 ms	$4.19 \cdot 10^{-15}$	820 ms	$4.23 \cdot 10^{-15}$
20	1.10 s	$1.04 \cdot 10^{-11}$	2.03 s	$6.41 \cdot 10^{-14}$	1.682 s	$5.66 \cdot 10^{-15}$	2.16 s	$5.72 \cdot 10^{-15}$
50	4.05 s	$1.06 \cdot 10^{-10}$	9.95 s	$6.04 \cdot 10^{-13}$	6.69 s	$6.18 \cdot 10^{-15}$	9.49 s	$6.38 \cdot 10^{-15}$
100	12.0 s	$4.77 \cdot 10^{-10}$	37.8 s	$3.29 \cdot 10^{-12}$	21.7 s	$7.82 \cdot 10^{-15}$	31.2 s	$7.87 \cdot 10^{-15}$

the algorithms. Triple Gram-Schmidt performs almost exactly as well as double Gram-Schmidt in terms of error, which is not surprising. It was stated during the lecture that the best result possible to achieve using multiple Gram-Schmidt is indeed obtained for double Gram-Schmidt. Note however that the CPU time required for triple Gram-Schmidt of course is considerably larger than for double Gram-Schmidt. The orthogonalization errors for the modified Gram-Schmidt is smaller than for single Gram-Schmidt but the algorithm is in this example seen to be worse than double Gram-Schmidt both in terms of CPU time and orthogonalization error.

3 Task 4

We investigate a primitive version of the Arnoldi method. Let K_m be a matrix representing the Krylov subspace:

$$K_m = [b, Ab/\|Ab\|, \dots, A^{m-1}b/\|A^{m-1}b\|] \in \mathbb{R}^{n\times m}. \tag{2}$$

3.1 (a)

The equation

$$\mu K_m^T K_m w = K_m^T A K_m w \tag{3}$$

is stemming from the Galerking method applied to the bilinear form associated with the eigenvalue problem $a(u,v) = u^T Av - \mu u^T v$, *with* $f(v) = 0$. *Prov that* (3) *is identical to the approximation generated by Arnoldi's method for eigenvalue problems.* The Arnoldi method computes an orthogonal basis of K_m such that after m iterations

$$AQ_m = Q_{m+1} H_{\underline{m}}, \tag{4}$$

where Q_m is an orthogonal matrix of size m and $H_{\underline{m}}$ is the corresponding Hessenberg matrix. The eigenvalues of A can then be approximated by the eigenvalues of

$$Q_m^T A Q_m. \tag{5}$$

We use the QR-factorisation of the matrix K_m, such that $K_m = Q_m R$. We first show that $R^T R = K_m^T K_m$. Using orthogonality, we have

$$I = Q_m^T Q_m. \tag{6}$$

Multiplying both sides of (6) with R^T and R respectively yields

$$\begin{aligned} R^T = R^T Q^T Q_m = K_m^T Q_m \Leftrightarrow \\ R^T R = K_m^T Q_m R = K_m^T K_m. \end{aligned} \tag{7}$$

Now, considering (3), we have

$$\begin{aligned} \mu K_m^T K_m w = K_m^T A K_m w \Leftrightarrow \\ \mu R^T R w = K_m^T A K_m w. \end{aligned} \tag{8}$$

Replacing K_m and K_m^T with the QR-factorisation of K_m yields

$$\mu R^T R w = R^T Q_m^T A Q_m R w. \tag{9}$$

Using that R is non-singular, we obtain

$$\mu w = Q_m^T A Q_m w. \tag{10}$$

Thus, the approximation computed from (3) is identical to the eigenvalue approximation obtained from (5), which is what we wanted to show.

3.2 (b)

We compare the eigenvalues computed using the Arnoldi method to eigenvalues computed using (3) after m iterations. Double Gram-Schmidt is used for orthogonalization and the matrix from task 3 is used with $nn = 12$ along with a random starting vector b. The result is visualised in Figure 1.

`eigenArnoldi.png`

Figure 1: Comparison of eigenvalues after m iterations.

3.3 (c)

In exact arithmetic we expect the results from the two approaches to agree. However, forming the Krylov matrices K_m for larger m gives close to singular matrices. As a result of bad conditioning, the Arnoldi approach is to prefer for computing the eigenvalues of the matrix.

4 Task 6

test

5 Task 7

test $\lambda_1 = -47.016 + i0.166$ $\lambda_2 = 1.314 + i12.664$ $\lambda_3 = 0.986 - i11.898$

$$\varepsilon_i^{(m)} \leq \frac{\rho^{m-1}}{|\lambda_i - c|^{m-1}}$$