SF3580
HW 2

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2018/11/29

1 Task 2

2 Task 4

The linear system of equations

$$\begin{bmatrix} 2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 2 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 2 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 2 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 2 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 2 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 2 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 2 \end{bmatrix} x = \begin{bmatrix} 1 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \tag{1}$$

is considered.

2.1 (a)

We determine the constants α, β and γ such that for the iterates $x_0, \dots x_3$ of the conjugate gradient method we obtain $\text{span}(x_0, x_1, x_2, x_3) = \text{span}(c_0, c_1, c_2, c_3)$, where

$$C = [c_0, c_1, c_2, c_3] = \begin{bmatrix} 1 & \alpha & 0 & \gamma \\ 1 & 0 & \beta & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 7 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}. \tag{2}$$

For this purpose, we use Lemma 2.2.4 from the lecture notes, stating that

$$\text{span}(b, Ab, \dots A^{m-1}b) = \text{span}(x_0, x_1, \dots, x_m). \tag{3}$$

Thus, we want to compute α, β and γ such that

$$\text{span}(b, Ab, A^2b, A^3b) = \text{span}(c_0, c_1, c_2, c_3). \tag{4}$$

We can directly conclude that $\text{span}(b) = \text{span}(c_0)$. Next, we want to make sure that $\text{span}(b, Ab) = \text{span}(c_0, c_1)$. By column reduction we thus find that $\alpha = 0$. Using that $\text{span}(b, Ab, A^2b) = \text{span}(c_0, c_1, c_2)$, we can similarly find that $\beta = -1$ and finally, using (4), and again reduce columns, we identify that $\gamma = 6$.

2.2 (b)

See the implemented Julia code. We have replaced `???` with $\|Ax - b\|_{A^{-1}}$. Comparing $\mathtt{x_{opt}}$ and $\mathtt{x_{cg}}$, we obtain a difference of $1.51 \cdot 10^{-11}$.

2.3 (c)

For GMRES, `???` is replaced by $\|Ax - b\|_2$. Now, comparing $\mathtt{x_{opt}}$ with $\mathtt{x_{gmres}}$, we obtain the difference $1.06 \cdot 10^{-11}$.

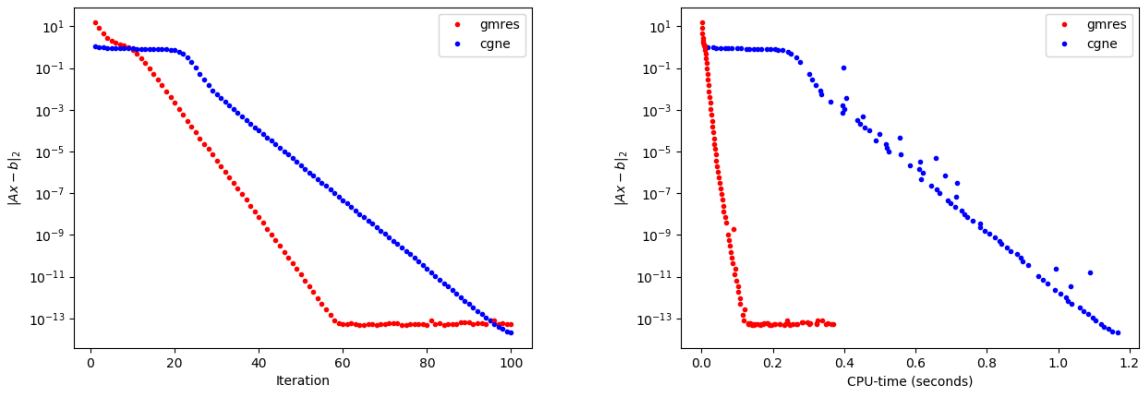
3 Task 5

Given a real symmetric matrix A with eigenvalues 10, 10.5 and 100 eigenvalues in the interval $[2, 3]$, we prove a bound for then number of steps needed for CG to reduce the error measured in $\|Ax_n - b\|_{A^{-1}} = \|x_n - x_*\|$ by a factor 10^7. We assume exact arithmetic and no breakdown.

4 Task 6

4.1 (a)

We compare GMRES and CGN for a given matrix B and right hand side b. The result of the comparison is visualised in Figure 1. The iterates of CGN span a different Krylov subspace than gmres and it is



(a) Error versus number of iterations required for gmres and cgn for the given system.

(b) Error versus CPU-time required for gmres and cgn for the given system.

Figure 1

mentioned in the lecture notes on this topic that in most cases, this subspace has worse approximation properties than the usual Krylov subspace used for the gmres iterates. This correspond with what can be observed in Figure 1a.

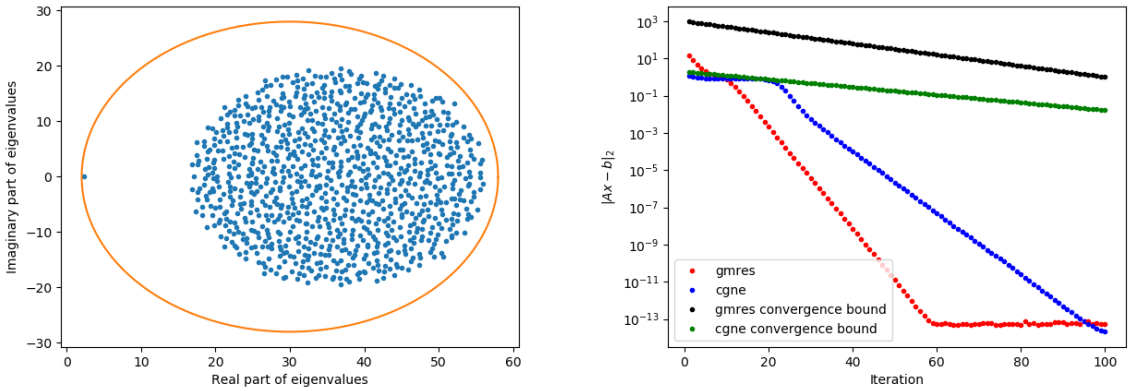
4.2 (b)

The result can be related to the convergence theory for CGN and GMRES. Investigating the eigenvalues of the matrix B, it is clear that all eigenvalues are contained in a disk, but for one isolated eigenvalue. However, trying to apply the convergence theory with two discs from the lecture notes is not possible in

this case, as the obtained convergence factor is larger than 1. Therefore, one large disc is used and we apply Corollary 2.1.5, choosing $r = 28$ and $c = 30$. The resulting disc and bound is found in Figure 2. Note that for both methods, the bound for the convergence factor is heavily overestimated.

For CGN, we use the condition number bound for the error in iteration m,

$$\frac{\|e_m\|_2}{\|e_0\|_2} \leq 2\left(\frac{\sqrt{K(B^TB)}-1}{\sqrt{K(B^TB)}+1}\right)^m \tag{5}$$



(a) Eigenvalues of the matrix B visualised together with disc of convergence used for gmres convergence estimate.

(b) Convergence for gmres and CGN along with estimates of their convergence factors.

Figure 2

5 Task 7

(a)

Given that $A = V^{-1}\Lambda V$ we want to show $A^k = A = V^{-1}\Lambda^k V$, which is done by induction. The initial stage is

$$A^2 = V^{-1}\Lambda V V^{-1}\Lambda V = V^{-1}\Lambda^2 V. \tag{6}$$

Assume $A^k = V^{-1}\Lambda^k V$ for some nonzero k, then

$$A^{k+1} = (V^{-1}\Lambda V)^k (V^{-1}\Lambda V) = V^{-1}\Lambda^k V\, V^{-1}\Lambda V = V^{-1}\Lambda^{k+1} V. \tag{7}$$

Thus $A^k = V^{-1}\Lambda^k V$. A simple consequence is that for $p \in P_n^0$ one has

$$p(A) = \sum_{k=1}^{n} a_k A^k = \sum_{k=1}^{n} a_k V^{-1}\Lambda^{k+1} V = V^{-1}\left(\sum_{k=1}^{n} a_k \Lambda^{k+1}\right) V = V^{-1} p\left(\Lambda^{k+1}\right) V \tag{8}$$

with $a_0 = 1$ for $p \in P_n^0$ and knowing that $A^0 = I$. We have

$$\min_{p\in P_n^0} \|p(A)\| \leq \|V\|\|V^{-1}\| \min_{p\in P_n^0} \|p(\Lambda)\| \tag{9}$$

as a consequence of norms being submultiplicative.

(b)

First we show by induction that

$$\begin{pmatrix} \lambda_1 & 1 \\ 0 & \lambda_1 \end{pmatrix}^k = \begin{pmatrix} \lambda_1^k & k\lambda_1^{k-1} \\ 0 & \lambda_1^k \end{pmatrix}. \tag{10}$$

The initial stage is for $k = 2$:

$$\begin{pmatrix} \lambda_1 & 1 \\ 0 & \lambda_1 \end{pmatrix}^2 = \begin{pmatrix} \lambda_1^2 & 2\lambda_1 \\ 0 & \lambda_1^2 \end{pmatrix}. \tag{11}$$

Assume (10) holds for k, then

$$\begin{pmatrix} \lambda_1 & 1 \\ 0 & \lambda_1 \end{pmatrix}^{k+1} = \begin{pmatrix} \lambda_1^k & k\lambda_1^{k-1} \\ 0 & \lambda_1^k \end{pmatrix} \begin{pmatrix} \lambda_1 & 1 \\ 0 & \lambda_1 \end{pmatrix} = \begin{pmatrix} \lambda_1^{k+1} & (k+1)\lambda_1^k \\ 0 & \lambda_1^{k+1} \end{pmatrix}, \tag{12}$$

i.e. the proposition (10) holds for all nonzero k.

Introduce the monomial $p_k(z) = z^k$, then

$$p_k\left(\begin{pmatrix} \lambda_1 & 1 \\ 0 & \lambda_1 \end{pmatrix}\right) = \begin{pmatrix} \lambda_1^k & k\lambda_1^{k-1} \\ 0 & \lambda_1^k \end{pmatrix} = \begin{pmatrix} p_k(\lambda_1) & p_k'(\lambda_1) \\ 0 & p_k(\lambda_1) \end{pmatrix} \tag{13}$$

which holds for all nonzero k from the induction proof above. We now have

$$p\left(\begin{pmatrix} \lambda_1 & 1 \\ 0 & \lambda_1 \end{pmatrix}\right) = \sum_{k=1}^{n} a_k p_k\left(\begin{pmatrix} \lambda_1 & 1 \\ 0 & \lambda_1 \end{pmatrix}\right) = \sum_{k=1}^{n} \begin{pmatrix} a_k p_k(\lambda_1) & a_k p_k'(\lambda_1) \\ 0 & a_k p_k(\lambda_1) \end{pmatrix} = \begin{pmatrix} p(\lambda_1) & p'(\lambda_1) \\ 0 & p(\lambda_1) \end{pmatrix}. \tag{14}$$

(c)

Let A be a block diagonal matrix, such that

$$A = \begin{pmatrix} A_1 & & & \\ & A_2 & & \\ & & \ddots & \\ & & & A_m \end{pmatrix} \tag{15}$$

where A_i are Jordan block matrices. Due to the block structure we have

$$p(A) = \begin{pmatrix} p(A_1) & & & \\ & p(A_2) & & \\ & & \ddots & \\ & & & p(A_m) \end{pmatrix}. \tag{16}$$

Each block $p(A_i)$ has a singular value decomposition $p(A_i) = U_i S_i V_H^*$, where U_i and V_i are unitary matrices. S_i is a diagonal matrix with the singular values σ as elements. We can now write $p(A)$ as follows.

$$p(A) = \underbrace{\begin{pmatrix} U_1 & & & \\ & U_2 & & \\ & & \ddots & \\ & & & U_m \end{pmatrix}}_{U:=} \underbrace{\begin{pmatrix} S_1 & & & \\ & S_2 & & \\ & & \ddots & \\ & & & S_m \end{pmatrix}}_{S:=} \underbrace{\begin{pmatrix} V_1^H & & & \\ & V_2^H & & \\ & & \ddots & \\ & & & V_m^H \end{pmatrix}}_{V^H:=} \tag{17}$$

due to the rules of multiplication for block diagonal matrices. The final result follows from the definition of the operator norm $\|\cdot\|_2$:

$$\begin{aligned}\|p(A)\|_2 &= \sigma_{\max}(p(A)) = \max S = \max_{i=1,\dots,m}(\max S_i)) \\ &= \max_{i=1,\dots,m}(\sigma_{\max}(p(A_i))) = \max_{i=1,\dots,m}(\|p(A_i)\|_2) \\ &= \max\left(\left\|\begin{pmatrix} p(\lambda_1) & p'(\lambda_1) \\ 0 & p(\lambda_1)\end{pmatrix}\right\|_2, |p(\lambda_3)|, \dots, |p(\lambda_m)|\right)\end{aligned}$$

(d)

It is clear that

$$p(z) = (\alpha_n + \beta_n z)\frac{(c-z)^{n-1}}{c^{n-1}} \tag{18}$$

satisfies $p \in P_n$. This immediately gives $\alpha_n = 1$. We now study

$$p'(z) = \frac{c\left(1-\frac{z}{c}\right)^n(\alpha_n - \alpha_n n + \beta_n(c-nz))}{(c-z)^2} = \frac{c\left(1-\frac{z}{c}\right)^n(1-n+\beta_n(c-nz))}{(c-z)^2}. \tag{19}$$

Thus

$$p'(\lambda_1) = 0 \Leftrightarrow \frac{c\left(1-\frac{\lambda_1}{c}\right)^n(1-n+\beta_n(c-n\lambda_1))}{(c-\lambda_1)^2} = 0 \Leftrightarrow (1-n+\beta_n(c-n\lambda_1)) = 0, \tag{20}$$

that is

$$\beta_n = \frac{n-1}{c-n\lambda_1}. \tag{21}$$

In turn this assumes that $c \neq n\lambda_1$ for $n > 1$.

(e)

Assuming x_n is the n:th iterate generated by GMRES-iterate, we have by lemma 2.1.3 from that lecture notes that

$$\begin{aligned}&\|Ax_n - b\|_2 = \min_{x\in\mathcal{K}n(A,b)}\|Ax-b\|_2 = \min_{p\in P_n^0}\|p(A)b\| \leq \|V\|\|V^{-1}\|\min_{p\in P_n^0}\|p(\Lambda)\|\|b\| \\ \Leftrightarrow &\frac{\|Ax_n - b\|_2}{\|b\|} \leq \|V\|\|V^{-1}\|\min_{p\in P_n^0}\|p(\Lambda)\|\end{aligned}$$

due to the result in 7 (a). Let

$$q(z) = \left(1 + z\frac{n-1}{c-n\lambda_1}\right)\frac{(c-z)^{n-1}}{c^{n-1}}. \tag{22}$$

from the previous task, which by construction is an element of P_n^0. Thus

$$\min_{p\in P_n^0}\|p(\Lambda)\| \leq \|q(\Lambda)\| = \max\left(\left\|\begin{pmatrix} q(\lambda_1) & q'(\lambda_1) \\ 0 & q(\lambda_1)\end{pmatrix}\right\|_2, |q(\lambda_3)|, \dots, |q(\lambda_m)|\right). \tag{23}$$

Recall that $q'(\lambda_1) = 0$ and that the matrix 2-norm of diagonal matrix is the largest element in modulus. The expression above can be simplified as

$$\min_{p\in P_n^0}\|p(\Lambda)\| \leq \max\left(|q(\lambda_1)|, |q(\lambda_3)|, \dots, |q(\lambda_m)|\right) = \max_{\lambda_i}\left(1 + \lambda_i\frac{n-1}{c-n\lambda_1}\right)\frac{(c-\lambda_i)^{n-1}}{c^{n-1}}. \tag{24}$$

It is given that all eigenvalues are contained in the disc centered at c with radius ρ. By taking the modulus the inequality (24) and assumin $\lambda_1 \neq 0$ we get

$$\min_{p\in P_n^0} \|p(\Lambda)\| \leq \max_{\lambda_i} \left|1 + \lambda_i \frac{n-1}{c - n\lambda_1}\right| \frac{\rho^{n-1}}{|c^{n-1}|} \leq \max_{\lambda_i} \frac{\overbrace{|c-\lambda_i|}^{\leq \rho} + n\overbrace{|\lambda_i - \lambda_1|}^{\leq 2\rho}}{|c - n\lambda_1|} \frac{\rho^{n-1}}{|c^{n-1}|} \leq \gamma_n \frac{\rho^n}{|c^n|}$$

with

$$\gamma_n = \frac{\frac{1}{n} + 2}{\left||\frac{1}{n}| - |\frac{\lambda_1}{c}|\right|}. \tag{25}$$

We already claimed that $c \neq n\lambda_1$, thus the denominator is nonzero for all n. In the limit we have

$$\lim_{n\to\infty} \gamma_n = 2\frac{|c|}{|\lambda_1|} \tag{26}$$

which is bounded. Combining all the results above gives

$$\frac{\|Ax_n - b\|_2}{\|b\|} \leq \|V\|\|V^{-1}\|\gamma_n \frac{\rho^n}{|c^n|}.$$

If $\lambda_1 = 0$ then $\beta_n = (n-1)/c$ and the corresponding bound for (24) is

$$\min_{p\in P_n^0} \|p(\Lambda)\| \leq \max_{\lambda_i} \left|1 + \lambda_i \frac{n-1}{c}\right| \frac{\rho^{n-1}}{|c^{n-1}|} \leq \max_{\lambda_i} \left(\overbrace{|c-\lambda_i|}^{\leq \rho} + n|\lambda_i|\right) \frac{\rho^{n-1}}{|c^n|} \leq \gamma_n \frac{\rho^n}{|c^n|}.$$

However, now

$$\gamma_n = \max_{\lambda_i} \left(1 + n\frac{|\lambda_i|}{\rho}\right), \tag{27}$$

which is not a bounded sequence.

(f)

For nonzero λ_1 we have convergence, but the speed is influenced by γ_n. Roughly, the further the centre c is from λ_1 the better. For many iterations we approximately get

$$\gamma_n \frac{\rho^n}{|c^n|} \approx \frac{2\rho}{|\lambda_1|} \frac{\rho^{n-1}}{|c^{n-1}|}. \tag{28}$$

Thus the rate of convergence is the same, but the factor $\frac{2\rho}{|\lambda_1|}$ may be large. So if the double eigenvalues lie close to zero and the other eigenvalues lies far away from the origin then the factor will be large.

For $\lambda_1 = 0$ the sequence γ_n is not bounded. Note that this does not mean that GMRES will diverge, only that the estimate gives no information.

(e)

We discussed with Aku Kammonen and Parikshit Upadhyaya.

References