

MAT 226B Large Scale Matrix Computation

Final Project

Ahmed Mahmoud

March, 22nd 2020

Problem 1:

(a) We know from nonsymmetric Lanczos process that

$$MV_k = V_k T_k + \beta_{k+1} [0 \dots 0 v_{k+1}]$$

We can multiply the above by e_1 to extract the first column (v_1) from V_k before multiplying it by M and the result is

$$\begin{aligned} MV_k e_1 &= V_k T_k e_1 + \beta_{k+1} [0 \dots 0 v_{k+1}] e_1 \\ MV_k e_1 &= V_k T_k e_1 + 0 \end{aligned}$$

Note that $MV_k e_1 = Mv_1$. Now, we can easily give the proof as

$$M^j r = M^j (\beta_1 v_1) = \beta_1 M^j v_1$$

$$M^j r = \beta_1 V_k T_k^j e_1, \quad \forall j = 0, 1, \dots, k-1 \quad (1)$$

For the second part, we note that $e_k^T T_k^{k-1} e_1 = 0$. Thus, the second sum has no effect. We can let $j = k$ in 1 and we get

$$M^k r = \beta_1 V_k T_k^k e_1 + \beta_1 \beta_{k+1} (e_k^T T_k^{k-1} e_1) v_{k+1}$$

(b) We follow the same steps as in (a). First we have

$$\begin{aligned} M^T W_k &= W_k \hat{T}_k + \gamma_{k+1} [0 \dots 0 w_{k+1}] \\ M^T W_k e_1 &= W_k \hat{T}_k e_1 + \gamma_{k+1} [0 \dots 0 w_{k+1}] e_1 \\ M^T w_1 &= W_k \hat{T}_k e_1 + 0 \end{aligned}$$

Taking the transpose of the above, we get

$$(M^T w_1)^T = w_1^T M = e_1^T \hat{T}_k^T W_k^T$$

We also know that $\hat{T}_k^T = D_k T_k D_k^{-1}$. Thus,

$$w_1^T M = e_1^T D_k T_k D_k^{-1} W_k^T$$

Now, we can give the proof as

$$\begin{aligned} c^T M^j &= \gamma_1 w_1^T M^j \\ c^T M^j &= \gamma_1 e_1^T D_k T_k^j D_k^{-1} W_k^T \\ c^T M^j &= \gamma_1 \delta_1 e_1^T T_k^j D_k^{-1} W_k^T \end{aligned}$$

(c) We can write the $Z(s)$ as

$$Z(s) = \sum_{j=0}^{\infty} \sigma^j c^T M^j r \tag{2}$$

We can find two values positive j_1 and j_2 such that $j_1 + j_2 = j$. Then, we can write 2 as

$$\begin{aligned} Z(s) &= \sum_{j=0}^{\infty} \sigma^j c^T M^{j_1} M^{j_2} r \\ Z(s) &= \sum_{j=0}^{\infty} \sigma^j (\gamma_1 \delta_1 e_1^T T_k^{j_1} D_k^{-1} W_k^T) (\beta_1 V_k T_k^{j_2} e_1) \end{aligned}$$

$$Z(s) = \sum_{j=0}^{\infty} \sigma^j \gamma_1 \delta_1 \beta_1 e_1^T T_k^{j_1} D_k^{-1} W_k^T V_k T_k^{j_2} e_1 \tag{3}$$

We know from Lanczos process that $W_k V_k = D_k$. In addition, we have $c^T r = (\gamma_1 w_1)^T (\beta_1 v_1) = \gamma_1 \beta_1 w_1^T v_1 = \gamma_1 \delta_1 \beta_1$. We can plug this relations in 3 to get

$$\begin{aligned} Z(s) &= \sum_{j=0}^{\infty} \sigma^j(c^T r) e_1^T T_k^{j_1} D_k^{-1} D_k T_k^{j_2} e_1 \\ Z(s) &= \sum_{j=0}^{\infty} \sigma^j(c^T r) e_1^T T_k^{j_1} T_k^{j_2} e_1 = \sum_{j=0}^{\infty} \sigma^j(c^T r) e_1^T T_k^j e_1 \end{aligned}$$

Problem 2:

Here we are required to find an efficient way to compute $q = Mv$ and $q = M^T v$ for $v \in \mathbb{C}^n$ where $M = (A - s_0 E)^{-1} E$. We can compute the matrix-vector multiplication efficiently using LU factorization. We first can write the multiplication as

$$\begin{aligned} q &= (A - s_0 E)^{-1} E v = \underbrace{(A - s_0 E)^{-1}}_W \underbrace{E v}_f \\ q &= W^{-1} f \Rightarrow W q = f \Rightarrow \underbrace{P D^{-1} W Q}_{LU} \underbrace{Q^T q}_d = P D^{-1} f \end{aligned}$$

Thus, we can first solve $Lc = P D^{-1} f$ for $c \in \mathbb{C}^n$ via forward substitution, then solve $Ud = c$ for $d \in \mathbb{C}^n$ via backward substitution, and finally set $q = Qd$.

We can use the same LU factorization to compute $q = M^T v$ efficiently. We first note that transposing the LU factorization for a given matrix W is $U^T L^T = Q^T W^T D^{-T} P^T$. We can write this multiplication as

$$\begin{aligned} q &= ((A - s_0 E)^{-1} E)^T v = E^T \underbrace{(A - s_0 E)^{-T} v}_g \\ g &= W^{-T} v \Rightarrow W^T g = v \Rightarrow \underbrace{Q^T W^T D^{-T} P^T}_{U^T L^T} \underbrace{(D^{-T} P^T)^{-1} g}_d = Q^T v \end{aligned}$$

Thus, we can first solve $U^T c = Q^T v$ for c via forward substitution, then solve $L^T d = c$ for d via backward substitution, and then set $g = D^{-T} P^T d$. Finally, we multiply g from the left by E^T to get q . The functions `Mv` and `transposeMv` implements these operations as discussed.

Problem 3:

The leading $2k$ moments $\mu_j = c^T M^j r$ for $j = 0, 1, \dots, 2k - 1$ can be computed as follows. Let $f_j = M^j r$. It is easy to see that $f_j = M f_{j-1}$ from which we can compute the moment at j as $\mu_j = c^T f_j$ and compute f_j recursively. We can use the same LU factorization to compute r and used the function `Mv` to compute f_j . The function `computeMoments` compute the moments as discussed here.

We wrote another function `textbookAlgo` that utilizes `computeMoments` to implement the textbook algorithm for computing $Z_k(s)$. More precisely, it compute the coefficient of the polynomials $p(\sigma)$ and $q(\sigma)$ such that $Z_k(s) = \frac{p(\sigma)}{q(\sigma)}$ where $p(\sigma) = \alpha_0 + \alpha_1\sigma + \dots + \alpha_{k-1}\sigma^{k-1}$, $q(\sigma) = \beta_0 + \beta_1\sigma + \dots + \beta_k\sigma^k$, $\alpha_0, \dots, \alpha_{k-1}, \beta_1, \dots, \beta_k \in \mathbb{C}$, and $\beta_0 = 1$. The output of this function is two vectors α and β containing the coefficients.

Problem 4:

We wrote the function `zkViaLanczos` which computes Z_k given T_k , s and s_0 . T_k is computed from our previous implementation of the nonsymmetric Lanczos in Homework 3 which feed in with the efficient implementation of the Mv and $M^T v$ from Problem 2.

System Specs: All our experiments run on Intel(R) Xeon(R) CPU E3-1280 v5 with 3.70 GHz and 32 GB of RAM on 64-bit operating system running Windows 7.

s_0 with fast convergence: We test our implementation of the textbook and Lanczos-based algorithm for different values of s_0 and found that it runs fairly fast for the small input given in `FP_Ex1.mat`; it takes less than a second even for large i.e., $k < 100$.

We followed the recommendation given in the lectures for how to pick s_0 . We choose $s_0 = 1e5 + 2\pi i 5.5e8$.

Comparison: We run both our implementation for different values of k and the above s_0 and compared between both. Table ?? should the average different ($\|\cdot\|^2$) and the maximum different between the two vectors containing the output of both algorithms for different values of s .

Explanation: We believe the reason why the textbook algorithm does not perform well is because it depends on computing $M^j r$ (to compute the moments) for increasing values of j which convergences quickly to the the eigenvector of M with largest eigenvalue. Thus, the information it contains comes from a single eigenvector where the information should comes from all eigenvectors of M . In contrast, Lanczos's T_k represents oblique projection of M onto the $K_k(M, r)$ Krylov subspace which contains information about k eigenvectors.

Problem 5:

(a)