Mehods of Computational Physics

Ayush Paliwal

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Problem Sheet 5 - Matrix Diagonalization

a) and b)
For example purpose, I am displaying an 8x8 matrix. A is my real symmetric matrix and T is its tridiagonal form. Each and every element is between [-1,1]. The matrix A satisfies $A = QTQ^T$, where Q is a orthonormal matrix.

$$A = \begin{pmatrix} -0.0888 & -0.3481 & 0.3777 & -0.4464 & 0.1906 & -0.1170 & -0.2466 & 0.2762 \\ -0.3481 & -0.7211 & 0.3231 & 0.6988 & 0.0645 & -0.6771 & -0.0217 & 0.4475 \\ 0.3777 & 0.3231 & -0.5908 & -0.3332 & -0.7628 & 0.0116 & 0.4085 & -0.3499 \\ -0.4464 & 0.6988 & -0.3332 & -0.5535 & 0.5234 & 0.5754 & -0.5413 & 0.1969 \\ 0.1906 & 0.0645 & -0.7628 & 0.5234 & -0.1639 & -0.0333 & -0.0378 & 0.3867 \\ -0.1170 & -0.6771 & 0.0116 & 0.5754 & -0.0333 & -0.1793 & -0.2894 & 0.4283 \\ -0.2466 & -0.0217 & 0.4085 & -0.5413 & -0.0378 & -0.2894 & 0.6602 & -0.1849 \\ 0.2762 & 0.4475 & -0.3499 & 0.1969 & 0.3867 & 0.4283 & -0.1849 & 0.4725 \end{pmatrix}$$

$$T = \begin{pmatrix} -0.0888 & 0.8063 & -0.0000 & -0.0000 & -0.0000 & -0.0000 & -0.0000 & 0.0000 \\ 0.8063 & -0.8508 & 0.5825 & -0.0000 & -0.0000 & -0.0000 & 0.0000 & -0.0000 \\ -0.0000 & 0.5825 & -0.7014 & -0.7668 & -0.0000 & -0.0000 & 0.0000 & 0.0000 \\ -0.0000 & -0.0000 & -0.7668 & -0.0613 & -1.4833 & 0.0000 & 0.0000 & 0.0000 \\ -0.0000 & -0.0000 & 0.0000 & -1.4833 & -0.2136 & 0.8008 & 0.0000 & 0.0000 \\ -0.0000 & -0.0000 & -0.0000 & 0.0000 & 0.8008 & 0.1657 & -0.1994 & -0.0000 \\ -0.0000 & 0.0000 & 0.0000 & -0.0000 & 0.0000 & -0.1994 & 0.4520 & 0.0973 \\ 0.0000 & -0.0000 & 0.0000 & 0.0000 & 0.0000 & -0.0000 & 0.0973 & 0.1333 \end{pmatrix}$$

Eigenvalues of A							
-2.066632033715121	-1.5298	1.6919	-0.5983	0.5908	0.4917	0.1723	0.0832
Eigenvalues of T							
-2.066632033715122	-1.5298	1.6919	-0.5983	0.5908	0.4917	0.1723	0.0832

Eigenvalues of A							
-2.066632034778399	-1.5298	-0.5983	0.0832	0.1723	0.4917	0.5908	1.6919
Eignevalues (Lanczos)							
-2.066632034778397	-1.5298	-0.5983	0.0832	0.1723	0.4917	0.5908	1.6919

$$Q=\begin{pmatrix} 1.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\ -0.0000 & -0.2183 & 0.2072 & 0.0788 & -0.8981 & 0.0635 & 0.2981 & -0.0601 \\ -0.0000 & -0.3437 & -0.4954 & 0.1164 & 0.0679 & -0.5993 & 0.3130 & -0.4014 \\ -0.0000 & 0.2839 & -0.2960 & -0.7771 & -0.0640 & 0.2506 & 0.3257 & -0.2342 \\ -0.0000 & 0.2519 & -0.7598 & 0.2785 & -0.3165 & 0.2007 & -0.3161 & 0.2033 \\ -0.0000 & 0.4767 & 0.1987 & -0.0768 & -0.2403 & -0.4117 & -0.5048 & -0.4952 \\ -0.0000 & -0.2735 & -0.0130 & 0.2262 & 0.1165 & 0.5989 & -0.1665 & -0.6884 \\ -0.0000 & -0.6230 & -0.0837 & -0.4916 & -0.1148 & -0.0743 & -0.5697 & 0.1412 \end{pmatrix}$$

One can show $A = QTQ^T$, easily:)

Now with increase in matrix size, we observe -

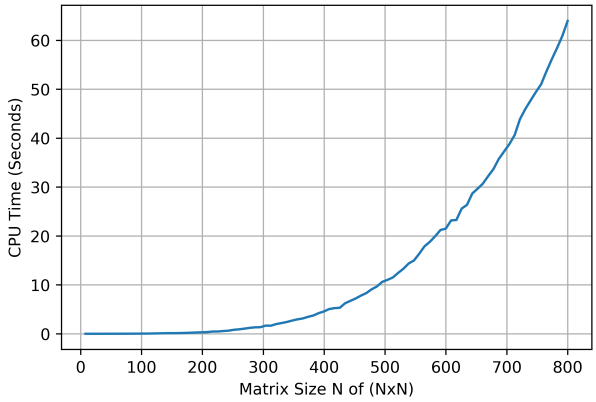

Figure 1: CPU time to compute T and eigenvalues for different matrix sizes. Matrix size varies from 8 to 800 in steps of 10

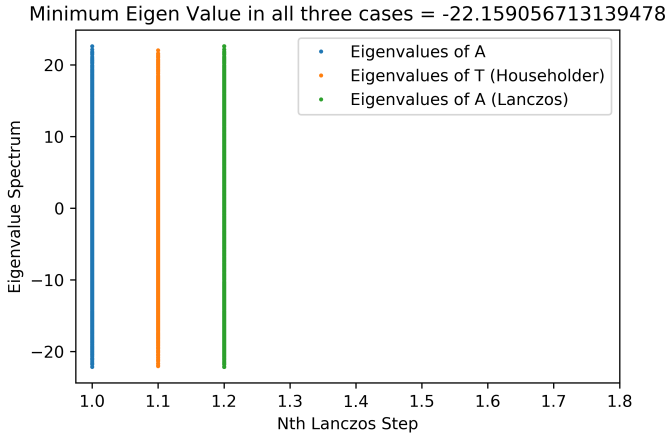

Figure 2: Estimate for the smallest eigenvalue using A, T and T(via Lanczos). A is 752x752

Lanczos Method

a)For the 8x8 matrix A used in first part of this problem sheet, the minimum eigenvalue (-2.066632034778) of matrix A matches via both the methods.
Lanczos Algorithm - An abstract concept of Kryov spaces is considered. A kryov space K(v,A):= $v, Av, A^2c, ...A^{n-1}v$ is defined in which the matrix A is tridiagonal. These orthonormal vectors are chosen as -
1. Choose arbitrary normalized vector ψ_o of dimension of n. A is nxn.
2. Define $\tilde{\psi}_1 = A\psi_o - a\psi_o$, where $a = A_{00}$
3. Next, $\tilde{\psi}_2 = A\psi_1 - a\psi_1 - b\psi_o$, where b=$||\psi_o||$
4. Iterate

b)

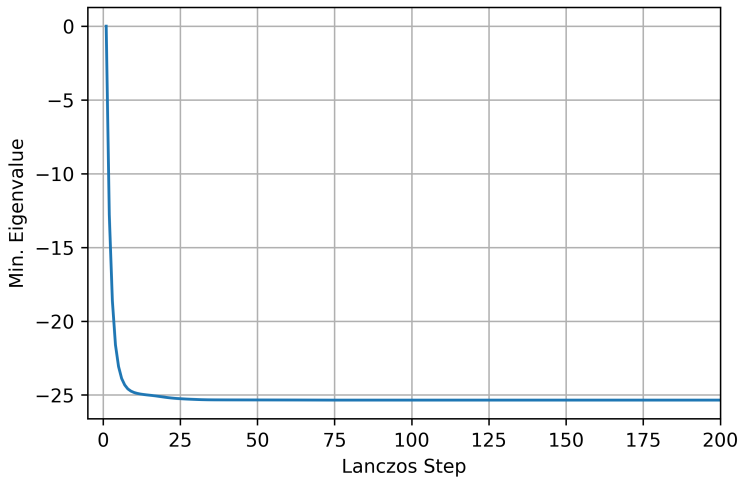

Figure 3: Estimate for the smallest eigenvalue with iteration. A is 1000x1000.

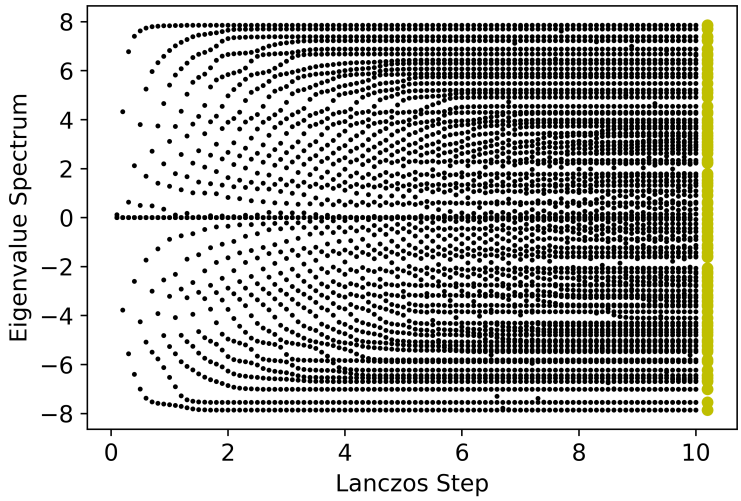

Figure 4: Estimation of eigenvalues at each Lanczos step. A is 100x100.

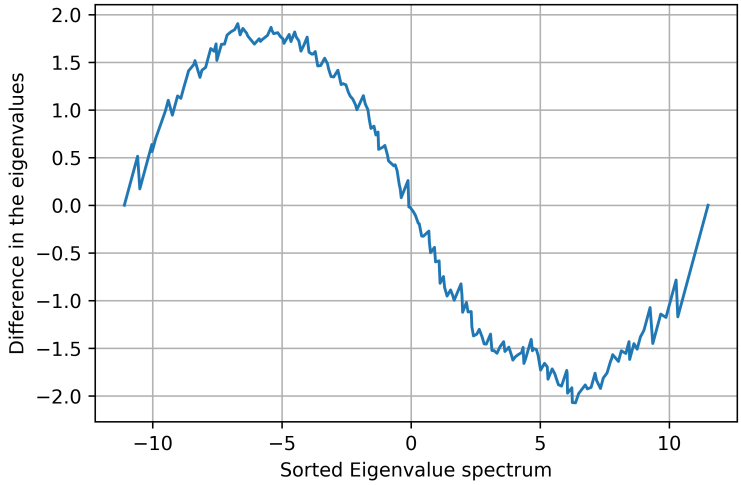

Figure 5: Estimate for larger eigenvalues. Intermediary eigenvalues suffer deviation on comparison.A is 200x200.

Estimate for larger eigenvalues can be judged from figure 5, which depicts that the largest and the lowest eigenvalue match via the **two methods**. The in-between eigenvalues vary.

c)

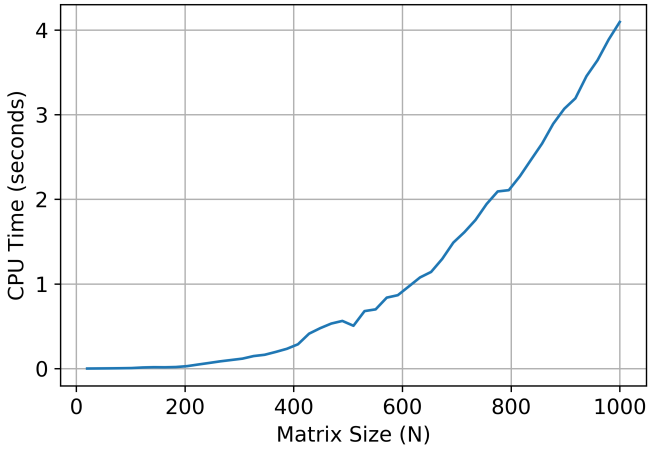

Figure 6: Plot for the CPU Time. Matrix size vary from 1 to 1000 in steps of 20

d) The Lanczos method can be used for very very large matrices but the drawback is, that it tends to give many false eigenvalues making it numerically unstable. This fact can be seen in the figure below and from figure 5 -

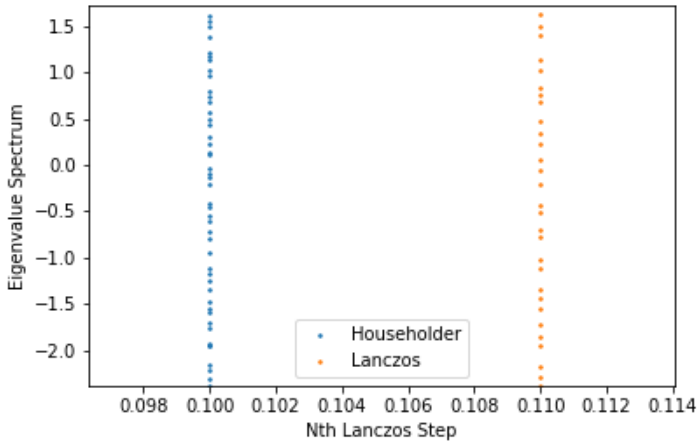

Figure 7: Eigenvalue spectrum for 200x200 matrix

One can see displaced dots for the two methods. These false eigenvalues

or the deviations become significant after n>30. But the largest and least eigenvalues always match via the two methods.
And if one is concerned only about the maximum and minimum eigenvalue, then I think it depends on ones CPU and RAM size.