Notes on numerical simultaneous matrix diagonalization

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Suppose we are given a set $\{A_j\}$ of N matrices $A_j \in \mathbb{C}^{MxM}$, where $j \in \{1,..,N\}$ and $N, M \in \mathbb{N}$. Provided that all matrices in this set pairwise commute with each other it is possible to find a common eigenbasis, which is characterized by $V \in \mathbb{C}^{MxM}$, such that $V^{-1}A_jV = D_j$ is diagonal $\forall j$. The purpose of the program is to numerically solve for the eigenvector matrix V and eigenvalues D_j.

Algorithm: We assume pairwise commutativity for the whole set of matrices, $[A_i, A_j] = A_iA_j - A_jA_i = 0\,\forall i, j \in \{1,..,N\}$. Further let all A_j be diagonalizable. We can then write $A_1 = U_1D_1U_{-1}$, or equivalently $D_1 = U_1^{-1}A_1U_1$. With the eigenvector matrix U_1 at hand we define $A_j^{(1)} = U_1^{-1}A_jU_1$ for $j \in \{2,..,N\}$. In the next stef we find the eigenvalue decomposition $D_2 = U_2^{-1}A_2^{(1)}U_2$ and update $A_j^{(2)} = U_2^{-1}A_j^{(1)}U_2$ accordingly. This procedure is continued until we reach $D_N = U_NA_N^{(N-1)}U_N$. The common eigenbasis is then found as $V = U_1 \cdot .. \cdot U_N = \prod_{j=1}^{N} U_j$, while the eigenvalues are $D_j = V^{-1}A_jV$.

An example in $\mathbb{R}^{2x2}$: We choose the set $\{A_1, A_2\}$, i.e. $N = 2$ with

$$A_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 1 & 0 & 2 \end{pmatrix} \;,\; A_2 = \begin{pmatrix} 2 & 4 & 0 \\ 3 & 1 & 0 \\ -1 & -4 & 1 \end{pmatrix} \;.$$

The diagonalization of A_1 gives $D_1 = U_1^{-1}A_1U_1$ where

$$U_1 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix} = U_1^{-1} \;.$$

Now we need to renormalize A_2 as

$$A_2^{(1)} = U_1^{-1}A_2U_1 = \begin{pmatrix} 2 & -4 & 0 \\ -3 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \;.$$

The second diagonalization then gives $D_2 = U_2^{-1}A_2^{(1)}U_2$ with

$$U_2 = \begin{pmatrix} 1 & 0 & -4 \\ 1 & 0 & 3 \\ 0 & 1 & 0 \end{pmatrix} \;,\; U_2^{-1} = \frac{1}{7}\begin{pmatrix} 3 & 4 & 0 \\ 0 & 0 & 7 \\ -1 & 1 & 0 \end{pmatrix} \;.$$

The common eigenbasis is then given by

$$V = U_1U_2 = \begin{pmatrix} -1 & 0 & 4 \\ 1 & 0 & 3 \\ 1 & 1 & -4 \end{pmatrix} \;,\; V^{-1} = U_2^{-1}U_1^{-1} = \frac{1}{7}\begin{pmatrix} -3 & 4 & 0 \\ 7 & 0 & 7 \\ 1 & 1 & 0 \end{pmatrix} \;.$$

From here we can find the eigenvalues from

$$D_1 = V^{-1} A_1 V = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 1 \end{pmatrix} \;, \; D_2 = V^{-1} A_2 V = \begin{pmatrix} -2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 5 \end{pmatrix} \;,$$

which concludes our small practical example.

Comments on the implementation Numerically it is important to catch the case of A_i and A_j, $i \neq j$, sharing common eigenvectors. In such a situation, assuming $i < j$, the matrix $A_j^{(i)}$ has already a diagonal form and it can be numerically unstable to diagonalize it once more (mainly due to rounding errors/numerical inaccuracies). The same holds true for all A_j, $j > 1$, that are diagonal from the beginning. This problem can be treated by simply skipping the diagonalization of any matrix that is diagonal up to numerical accuracy.

MATLAB code: Created with version R2013b, expected to be compatible with newer versions.