Project: Diagonalization of matrix with power method and Gram-Schmidt orthogonalization

Tomasz Chwiej

8th April 2025

1 Introduction

Diagonaliazation of symmetric matrix can be performed iteratively with the power method which always looks for an eigenvector having an eigenvalue of largest magnitude. In order to find another eigenvector one needs to remove from the vector contributions from already determined eigenvectors what is done by Gram-Schmidt orthogonalization. As for every iteration process we need to limit the maximum allowed iteration (variable *itmax*) and additional stopping criterion (variable ε) in case the wanted eigenvalue converges at iteration $it < itmax$. Simple algorithm for an improved power method with embedded orthogonalization process may look as follows

initialization: n, $A \in R^{n\times n}$, ε, itmax
for k=0 to n-1 by 1 do
    !fill starting vector $\vec{x}$ with random numbers:
        $(\vec{x})_i \leftarrow (double)rand()/RAND\_MAX, \quad i = 0, 1, \ldots, n-1$
    !initialize buffer eigenvalue with large number:
        $\lambda_{old} \leftarrow 10^5$
    !iterate until one of stopping critteria will be fulfilled
    for it=1 to itmax by 1 do
        !calculate new approximation:
            $\vec{y} \leftarrow A\vec{x}$
        !estimate eigenvalue:
            $\lambda \leftarrow \frac{\vec{x}^T(A\vec{x})}{\vec{x}^T\vec{x}}$
        !conduct Gram-Schmidt orthogonalization:
            $\vec{y} \leftarrow P_{GS}\,\vec{y} = \left(I - \sum_{m=0}^{k-1} \vec{x}_m\vec{x}_m^T\right)\vec{y}$
        !normalize vector & save for next iteration:
            $\vec{x} \leftarrow \frac{\vec{y}}{\|\vec{y}\|_2}$
        !check stopping criterion:
            $if\left(\left|\frac{\lambda-\lambda_{old}}{\lambda_{old}}\right| < \varepsilon\right) break$
        !save new eigenvalue approximation for next iteration
            $\lambda_{old} \leftarrow \lambda$
    end do

    !save eigenvector & eigenvalue:
        $\vec{x}_k \leftarrow \vec{x}$

$\lambda_k \leftarrow \lambda$

```
end do
```

2 Practical part

Tasks to do

1. Write computer program for matrix diagonalization using an algorithm of the power method presented in Sec.1. Assume: $n = 6$, $itmax = 150$, $\varepsilon = 10^{-8}$, fill the matrix elements with values from finite difference approximation of second order differential operator $\frac{d^2 f_i}{dx^2} \approx \frac{f_{i+1}-2f_i+f_{i-1}}{\Delta^2}$, $\Delta = 1$, namely:
$$a_{i,j} = \begin{cases} -2 & \Longleftrightarrow & j = i \\ 1 & \Longleftrightarrow & j = i \pm 1 \\ 0 & \Longleftrightarrow & j \notin \{i-1, i, i+1\} \end{cases} \tag{1}$$
Nontheless the matrix is sparse (tridiagonal), declare matrix A as 2D array in your program, for such small matrix implementation of CSR is a waste of time.

2. Check if the matrix is filled properly, simply display it on a screen.

3. Iteratively find consecutive pairs of the eigenvalues and the eigenvectors. Save subsequent approximations of eigenvalues to separate file.

4. When the iterative process is accomplished reconstruct the matrix A as sum of rank(1) matrices composed of its eigenvectors and eigenvalues
$$A_{num} = \sum_{k=0}^{n-1} \lambda_k \vec{x}_k \vec{x}_k^T \tag{2}$$
and its inverse
$$A_{num}^{-1} = \sum_{k=0}^{n-1} \frac{1}{\lambda_k} \vec{x}_k \vec{x}_k^T \tag{3}$$
Save both matrices to file.

5. At home prepare the report including obtained results. Show the iteratively improved eigenvalues in one plot (dependence of eigenvalues on iteration index). Try to answear to the following questions
   - How the number of iterations, needed to get the convergence of particular eigenvalue, depends on the global index of this eigenvalue? Should we expect such behaviour always? Try to find 10 largest eigenvalues for larger matrix $n = 200$.
   - Does the reconstructed matrix A_{new} has the same entries as the original one? Check what will happen if we assume less restricitve criterion e.g. $\varepsilon = 10^{-4}$? Reconstruct the matrix A_{new} and look how the matrix elements will change.
   - Is the inverse matrix symmetric? Can you simply prove it should be symmetric (use definition of inverse matrix)?
   - What will happen if you turn off Gram-Schmidt orthogonalization? Are you able to find all eigenvectors?

3 Computational hints

In this project you don't need external numerical libraries, just write your own routine for scalar product of two vectors and routine for matrix vector multiplication. For Gram-Schmidt projector($\vec{y} \leftarrow P_{GS}\,\vec{y}$) removing from the k-th eigenvector contributions from already found $m = 0, 1, \dots, k-1$ eigenvectors just consider the following piece of code

```
for m=0 to k-1 by 1 do
        calculate scalar product:
                c = x_m^T y
        remove contribution originated  from x_m
                y <- y - c x_m
end do
```

$$c = \vec{x}_m^T \vec{y}, \qquad \vec{y} \leftarrow \vec{y} - c\vec{x}_m$$

For the first vector ($k = 0$) orthogonalization will be automatically skipped.

4 Example results

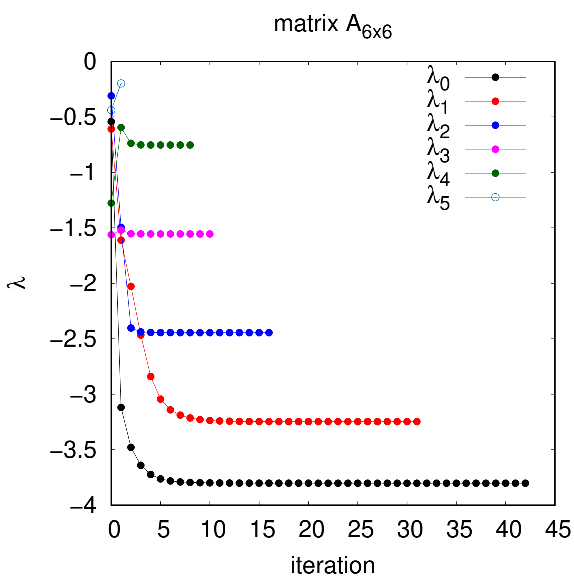

Figure 1: Example iterative approximations of eigenvalues for $n = 6$.