Mira Mors and Elias Tidemand Ruud

Computational Physics I FYS3150/FYS4150

Department of Physics University of Oslo Norway September 2020

Contents

1	Abstract	2
2	Introduction	2
3	Methods	2
	3.1 Jacobi Method	2

1 Abstract

2 Introduction

3 Methods

Since **U** is orthogonal holds $\mathbf{U}^{\mathbf{T}}\mathbf{U} = I$

$$w_i^T w_i = (Uv_i)^T (Uv_i) = v_i^T U^T U v_i = v_i^T I v_i = v_i^T v_i$$
 (1)

3.1 Jacobi Method

The Jacobi method guarantees a solution for all real symmetric matrices. The method rotates the initial matrix using similarity transformations. By discarding the off-diagonal elements, the eigenvalues stay preserved. How does this work? Firstly, we look at the transformation matrix.

The transformation matrix is orthogonal since its inverse is equal to its transpose

$$\mathbf{S}^T = \mathbf{S}^{-1}.$$

In \mathbb{R}^2 , the transformation matrix is given by

$$\begin{bmatrix} cos(\theta) & -sin(\theta) \\ sin(\theta) & cos(\theta) \end{bmatrix}$$

and θ denotes the degree of rotation in the plane.

In \mathbb{R}^3 , the rotation along the x, y and z axis respectively are

$$R_x = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos(\theta) & -\sin(\theta) \\ 0 & \sin(\theta) & \cos(\theta) \end{bmatrix} \qquad R_y = \begin{bmatrix} \cos(\theta) & 0 & -\sin(\theta) \\ 0 & 1 & 0 \\ \sin(\theta) & 0 & \cos(\theta) \end{bmatrix} \qquad R_z = \begin{bmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Generally, a rotation i \mathbb{R}^n is given by

$$S(k,l,\theta) = \begin{bmatrix} 1 & \dots & 0 & \dots & 0 & \dots & 0 \\ \vdots & \ddots & \vdots & & \vdots & & \vdots \\ 0 & \dots & \cos(\theta) & \dots & -\sin(\theta) & \dots & 0 \\ \vdots & & \vdots & \ddots & \vdots & & \vdots \\ 0 & \dots & \sin(\theta) & \dots & \cos(\theta) & \dots & 0 \\ \vdots & & \vdots & & \vdots & \ddots & \vdots \\ 0 & \dots & 0 & \dots & 0 & \dots & 1 \end{bmatrix}$$

 $cos(\theta)$ and $sin(\theta)$ are now placed in the lth row and lth column and kth row and kth column.

The similarity transformation

$$\mathbf{A}_{new} = \mathbf{S}^{T}(k, l, \theta) \cdot \mathbf{A} \cdot \mathbf{S}(k, l, \theta) \tag{2}$$

rotates row and column k and l of **A** an angle θ such as the entries $\mathbf{A}_{new}(k,l)$ and $\mathbf{A}_{new}(l,k)$ become zero.

The new entries are given with

$$b_{ii} = a_{ii} \quad i \neq k, i \neq l$$

$$b_{ik} = a_{ik}cos(\theta) - a_{il}sin(\theta) \quad i \neq k, i \neq l$$

$$b_{il} = a_{il}cos(\theta) + a_{ik}sin(\theta) \quad i \neq k, i \neq l$$

$$b_{kk} = a_{kk}cos^{2}(\theta) - 2a_{kl}cos(\theta)sin(\theta) + a_{l}lsin^{2}(\theta)$$

$$b_{ll} = a_{ll}cos^{2}(\theta) + 2a_{kl}cos(\theta)sin(\theta) + a_{kk}sin^{2}(\theta)$$

$$b_{kl} = (a_{kk} - a_{ll})cos(\theta)sin(\theta) + a_{kl}(cos^{2}(\theta) - sin^{2}(\theta))$$
(3)

The aim is to get zero for all non-diagonal elements b_{kl} . For each iteration, θ must be chosen accordingly. The Jacobi Method is an iterative method, thus this procedure is continued until the sum over the squared non-diagonal matrix elements, $off(\mathbf{A})$, are less than a prefixed test, ϵ , (ideally equal zero). That is

$$off(\mathbf{A}) = \sqrt{\sum_{i=1}^{n} \sum_{j=1, j \neq i}^{n} = |a_{ij}|^2} < \epsilon$$
 (4)

Since this is quite a time-consuming test, it can be replaced by finding the largest (absolute) value of the off-diagonal elements

$$max|a_{ij}| < \epsilon \quad i \neq j. \tag{5}$$

Even though $\mathbf{A}_{new}(k,l)$ and $\mathbf{A}_{new}(l,k)$ are set to zero for one iteration, these values can Given a real symmetric matrix, the algorithm is set to succeed. However, the large amount of iterations (about n^3) make the method very slow.