FYS4150: Project 2

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Unitary and orthogonal transformations (a)

A unitary matrix U has the properties:

$$U^{-1} = U^\dagger \tag{1}$$

An orthogonal matrix (the corresponding real matrix) has the properties:

$$U^T = U^{-1} \tag{2}$$

Where $U^\dagger$ is for matrices in Hilbert space (complex matrices). It represents the transpose of the complex conjugate, i.e. $U^\dagger = (U^*)^T$.

Assume we have an orthogonal basis for the n-dimensional space v_i, where $v_j^T v_i = \delta_{ij}$:

$$\mathbf{v}_i = \begin{bmatrix} v_{i1} \\ \dots \\ \dots \\ v_{in} \end{bmatrix} , \quad U\mathbf{v}_i = \mathbf{w}_i$$

Under orthogonal transformations, both the dot product and orthogonality of vectors is conserved:

$$\mathbf{w}_i^T \mathbf{w}_j = (U\mathbf{v}_i)^T (U\mathbf{v}_j) = \mathbf{v}_i^T U^T U \mathbf{v}_j = \mathbf{v}_i^T U^{-1} U \mathbf{v}_j = \mathbf{v}_i^T \mathbf{v}_j = \delta_{ij}$$

Jacobi's rotation method (b)

We want to solve the eigenvalue problem for a tridiagonal matrix:

$$
\begin{pmatrix}
d_0 & e_0 & 0 & \dots & 0 & 0 \\
e_1 & d_1 & e_1 & \dots & 0 & 0 \\
0 & e_2 & d_2 & e_2 & \dots & 0 \\
\vdots & & & \ddots & & 0 \\
0 & \dots & \dots & 0 & e_N & d_N
\end{pmatrix}
\begin{pmatrix}
u_0 \\
u_1 \\
\vdots \\
u_{N-1} \\
u_N
\end{pmatrix}
= \lambda
\begin{pmatrix}
u_0 \\
u_1 \\
\vdots \\
u_{N-1} \\
u_N
\end{pmatrix}
\tag{3}
$$

We want to use Jacobi's rotation method. We define an orthogonal matrix S to operate on our matrix A:

$$
B = S^T A S \tag{4}
$$

With all elements in S equal to zero, except:

$$
s_{kk} = s_{ll} = \cos\theta \ , \ s_{kl} = -s_{lk} = s\sin\theta \ , \ s_{ii} = 1 \ ; \ i \neq k \ i \neq l
$$

1. Find $\max(a_{kl})$.

2. Compute the rotation parameters $t = \tan\theta$, $c = \cos\theta$, $s = \sin\theta$:

$$
\tau = \cot\theta = \frac{a_{ll} - a_{kk}}{2a_{kl}} \tag{5}
$$

$$
t = -\tau \pm \sqrt{1 + \tau^2} \tag{6}
$$

$$
c = \frac{1}{1 + t^2} \ , \ s = tc \tag{7}
$$

3. Calculate the elements of B:

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

$$
b_{ik} = a_{ik}c - a_{il}s \ , \ i \neq k \ i \neq l
$$

$$
b_{il} = a_{il}c + a_{ik}s \ , \ i \neq k \ i \neq l
$$

$$
b_{kk} = a_{kk}c^2 - 2a_{kl}c*s + a_{ll}s^2
$$

$$
b_{ll} = a_{ll}c^2 + 2a_{kl}c*s + a_{kk}s^2
$$

$$
b_{kl} = (a_{kk} - a_{ll})c*s + a_{kl}(c^2 - s^2)
$$

4. If $\max(b_{kl}) \geq \epsilon$ run the algorithm again.

Figure 1: Jacobi rotation algorithm for tridiagonal matrix