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 $v_j^T v_i = \delta_{ij}$:

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

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:

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

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

Benchmarks

Jacobi rotation

Check the Jacobi function, which finds eigenvalues of a matrix, on the matrix A:

$$A = \begin{pmatrix} 1 & 2 & 0 \\ 2 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \ , \ \det(A - \lambda \mathbb{1}) = \begin{vmatrix} 1-\lambda & 2 & 0 \\ 2 & 1-\lambda & 0 \\ 0 & 0 & 1-\lambda \end{vmatrix}$$

$$\det(A - \lambda \mathbb{1}) = (1-\lambda)^3 - 2 \cdot 2(1-\lambda) = (1-\lambda)[(1-\lambda)^2 - 4]$$

$$= (1-\lambda)[\lambda^2 - 2\lambda - 3] \rightarrow \lambda = 1 \cap \lambda = 2$$

$$\rightarrow (\lambda - 1)(\lambda - 1)(\lambda - 2)$$