Task 8. QR method of the calculation of square matrix eigenvalues

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Task 8

Write a program that calculates all the eigenvalues of the square matrix **A** with the QR method.

Note that in this task "QR" appears in the context of two different methods

(1) Iterative QR method for the calculation of the matrix eigenvalues

(2) QR decomposition of the the matrix

Furthermore, QR method (1) uses QR decomposition (2)

Eigenvalue problem

- Eigenvalue equation for **A** square matrix $n \times n$

$$\mathrm{Ax} = \lambda \mathrm{x} \quad \Leftrightarrow \quad (\mathrm{A} - \lambda 1)\mathrm{x} = 0$$

x eigenvector ($n \times 1$), λ - eigenvalue (number, in general it may be complex number)

- Eigenvalues λ are the roots of the characteristic polynomial, i.e.

$$\det(\mathrm{A} - \lambda 1) = 0$$

- In particular, if $\mathbf{A} = \mathbf{U}$ is the (upper) triangular matrix, then

$$\det(\mathrm{U} - \lambda 1) = (u_{11} - \lambda)(u_{22} - \lambda)...(u_{nn} - \lambda) = 0$$

which means that $\lambda_i = u_{ii}$, where $i = 1, ..., n$

Similar matrices

- **Definition:** Matrices $\mathbf{A}$ and $\mathbf{B}$ are similar $\Leftrightarrow \exists\, \mathbf{C}\ \mathbf{B} = \mathbf{C}^{-1}\mathbf{AC}$, where $\det \mathbf{C} \neq 0$
- **Theorem:** Similar matrices possess the same eigenvalues
  Proof:

$$
\begin{aligned}
& \boldsymbol{A}\boldsymbol{x} = \lambda \boldsymbol{x} \\
\boldsymbol{C}^{-1} \cdot \big| \quad & \boldsymbol{A}1\boldsymbol{x} = \lambda \boldsymbol{x} \\
& \boldsymbol{C}^{-1}\boldsymbol{A}(\boldsymbol{C}\boldsymbol{C}^{-1})\boldsymbol{x} = \boldsymbol{C}^{-1}\lambda \boldsymbol{x} \\
& (\boldsymbol{C}^{-1}\boldsymbol{A}\boldsymbol{C})(\boldsymbol{C}^{-1}\boldsymbol{x}) = \lambda(\boldsymbol{C}^{-1}\boldsymbol{x}) \\
& \boldsymbol{B}\boldsymbol{x}' = \lambda \boldsymbol{x}',
\end{aligned}
$$

  where $\boldsymbol{x}' = \boldsymbol{C}^{-1}\boldsymbol{x}$

Orthogonal matrices - general properties

- **Definition:** Matrix Q $n \times n$ is orthogonal $\Leftrightarrow$

$$QQ^{Tr} = Q^{\mathrm{Tr}}Q = 1,$$

i.e. $Q^{Tr} = Q^{-1}$

- Matrix element $(QQ^{Tr})_{ij}$

$$(QQ^{Tr})_{ij} = \sum_{k=1}^{n} Q_{ik}(Q^{Tr})_{kj} = \sum_{k=1}^{n} Q_{ik}Q_{jk} = \delta_{ij}$$

Rows of the orthogonal matrix are orthonormal

- Matrix element $(Q^{\mathrm{Tr}}Q)_{ij}$

$$(Q^{\mathrm{Tr}}Q)_{ij} = \sum_{k=1}^{n} (Q^{Tr})_{ik}Q_{kj} = \sum_{k=1}^{n} Q_{ki}Q_{kj} = \delta_{ij}$$

Columns of the orthogonal matrix are orthonormal

QR method (1) for the calculation of matrix eigenvalues

- **Theorem** If the square real matrix **A** $n \times n$ possesses n different eigenvalues, i.e. $|\lambda_1| > |\lambda_2| > ... > |\lambda_n|$, then the sequence of A_k matrices converges to upper triangular matrix, where

$$A_1 = A$$
$$A_k = Q_k R_k \quad \text{rozkład QR}$$
$$A_{k+1} = R_k Q_k$$

Q_k - orthogonal matrix, R_k - upper triangular matrix

- Matrices A_k and A_{k+1} are similar

$$Q_k^{-1} \cdot | \quad A_k = Q_k R_k \quad \Rightarrow \quad R_k = Q_k^{Tr} A_k$$

$$A_{k+1} = R_k Q_k = Q_k^{Tr} A_k Q_k$$

Thus, matrices A_k, k=1,2,..., possess the same eigenvalues (as A)

- If real matrix A is symmetric, then the sequence of A_k matrices converges to diagonal matrix

QR decomposition (2): A = QR

Procedure uses Hauseholder transformations

- We construct subsequent matrices $\mathrm{A}^{(1)}$, $\mathrm{A}^{(2)}$, ... $\mathrm{A}^{(n)}$

$$\mathrm{A}^{(1)} = \mathrm{A}$$
$$\mathrm{A}^{(k+1)} = \mathrm{Q}^{(k)}\mathrm{A}^{(k)}, \quad k = 1, 2, \ldots, n-1.$$

- Symmetric and orthogonal Hauseholder matrix $\mathrm{Q}^{(k)}$

$$\mathrm{Q}^{(k)} = 1 - 2\mathrm{x}^{(k)}(\mathrm{x}^{(k)})^{Tr}, \quad (\mathrm{x}^{(k)})^{Tr}\mathrm{x}^{(k)} = 1$$
$$Q_{ij}^{(k)} = \delta_{ij} - 2x_i^{(k)}x_j^{(k)}, \quad i, j = 1, 2, \ldots, n$$

  are evaluated from the condition

$$A_{ik}^{(k+1)} = 0, \quad i = k+1, \ldots, n$$

- $\mathrm{x}^{(k)}$ is the normalized vector (column $n \times 1$)
- Matrix $\mathrm{A}^{(k+1)}$ possess zeros below the main diagonal in first k columns

G. Golub, W. Kahan, *Calculating the singular values and pseudo-inverse of a matrix*, J. SIAM Numer. Anal. B 2, 205-224 (1965).

Example of $A^{(6)}$ - almost triangular matrix

$$\begin{pmatrix} \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ 0 & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ 0 & 0 & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ 0 & 0 & 0 & \bullet & \bullet & \bullet & \bullet & \bullet \\ 0 & 0 & 0 & 0 & \bullet & \bullet & \bullet & \bullet \\ 0 & 0 & 0 & 0 & 0 & \bullet & \bullet & \bullet \\ 0 & 0 & 0 & 0 & 0 & \bullet & \bullet & \bullet \\ 0 & 0 & 0 & 0 & 0 & \bullet & \bullet & \bullet \end{pmatrix}_{8\times 8}$$

G. Golub, W. Kahan, *Calculating the singular values and pseudo-inverse of a matrix*, J. SIAM Numer. Anal. B 2, 205-224 (1965).

QR decomposition (2): $A = QR$

Calculation of normalized vectors $\mathrm{x}^{(k)}$

$$s_k = \sqrt{\sum_{i=k}^{n} |A_{ik}^{(k)}|^2}$$

$$x_i^{(k)} = 0, \quad i < k$$

$$x_k^{(k)} = \sqrt{\frac{1}{2}\left(1 + \frac{|A_{kk}^{(k)}|}{s_k}\right)}$$

$$x_i^{(k)} = c_k\, A_{i,k}^{(k)}, \quad i = k+1, \ldots, n$$

where

$$c_k = \frac{\mathrm{sign}(A_{kk}^{(k)})}{2 s_k\, x_k^{(k)}}$$

If $s_k = 0$, then $\mathrm{x}^{(k)} = 0$

G. Golub, W. Kahan, *Calculating the singular values and pseudo-inverse of a matrix*, J. SIAM Numer. Anal. B 2, 205-224 (1965).

QR decomposition (2): $A = QR$

$$A^{(1)} = A$$

$$A^{(k+1)} = Q^{(k)} A^{(k)}, \quad k = 1, 2, \ldots, n-1$$

$$\Downarrow$$

Orthogonal matrix

$$Q = Q^{(1)} Q^{(2)} \ldots Q^{(n-1)}$$

Upper triangular matrix

$$R = A^{(n)}$$

G. Golub, W. Kahan, *Calculating the singular values and pseudo-inverse of a matrix*, J. SIAM Numer. Anal. B 2, 205-224 (1965).

QR method (1) for the calculation of the matrix eigenvalues

- Algorithm

$$A_1 = A$$
$$A_k = Q_k R_k$$
$$A_{k+1} = R_k Q_k$$

- What is the condition for the end of iterations?
  - A_{k+1} is the upper triangular matrix
  - Diagonal elements of A_k of A_{k+1} are the same
  - In fact, the matrices A_k and A_{k+1} are the same
  - This means that Q_k is the matrix with $(Q_k)_{ij} = \pm\delta_{ij}$

  In practice, all the above conditions can be satisfied only approximately
- Eigenvalues of **A** matrix are the diagonal elements of the upper triangular matrix $A_{k_{max}}$
- If A is symmetric, then A_k is diagonal and the columns of orthogonal matrix $Q = Q_1 Q_2 \dots Q_{k_{max}}$ are the eigenvectors of A for the subsequent eigenvalues $\lambda_i = (A_k)_{ii}$, i.e.

$$Aq_i = \lambda_i q_i,$$

  where q_i is *i*-th column of Q matrix

TO DO

1. Read the real matrix $\mathbf{A}$ of the size $n \times n$ from the input
2. Calculate subsequent A_{k+1} matrices using QR decomposition of previous matrix A_k
3. Check $Q_k R_k = A_k$
4. Introduce conditions for the interruption of the iterations
5. Calculate eigenvalues for the symmetric and non-symmetric matrices
6. Check the convergence of the QR iterative method for the matrix, which possesses two the same eigenvalues
7. Compare the results with those obtained with existing functions (e.g. eig() in Matlab)

Examples

$$A = \begin{pmatrix} 1 & 1 & 1 \\ 2 & -2 & 2 \\ 3 & 3 & -3 \end{pmatrix}$$

$$A = \begin{pmatrix} 1 & 2 & 3 & 5 \\ 2 & 3 & 4 & 5 \\ 3 & 4 & 5 & 6 \\ 5 & 5 & 6 & 8 \end{pmatrix}$$

$$A = \begin{pmatrix} 2 & 13 & -14 & 3 \\ -2 & 25 & -22 & 4 \\ -3 & 31 & -27 & 5 \\ -2 & 34 & -32 & 7 \end{pmatrix}$$

Rozkład QR - inne podejście

- Kolumny
$$\mathrm{A} = [\mathrm{a}_1\ \mathrm{a}_2\ \dots\ \mathrm{a}_\mathrm{n}] \quad \mathrm{Q} = [\mathrm{q}_1\ \mathrm{q}_2\ \dots\ \mathrm{q}_\mathrm{n}],$$
gdzie a_k i q_k - k-te kolumny $(n \times 1)$ macierzy A i Q
- Norma wektora
$$\|\mathrm{v}\| = \|\mathrm{v}\|_2 = \sqrt{\sum_{j=1}^{n} v_j^2}$$
W szczególności $\|\mathrm{a}_k\| = \sqrt{\sum_{i=1}^{n} a_{ik}^2}$
- Iloczyn skalarny wektorów
$$\mathrm{u}^{\mathrm{Tr}}\mathrm{v} = \sum_{j=1}^{n} u_j v_j$$
W szczególności $\mathrm{q}_\mathrm{k}^{\mathrm{Tr}}\mathrm{a}_\mathrm{i} = \sum_{j=1}^{n} q_{jk} a_{ji}$

Rozkład QR - algorytm (mniej stabilny[1])

- Ortogonalizacja Grama-Schmidta kolumn macierzy A, tzn. $\{a_k\} \rightarrow \{q_k\}$, gdzie $q_i^{Tr} q_j = \delta_{ij}$
    1. $q_1 = \frac{a_1}{\|a_1\|}$
    2. $i = 2, \ldots n$

$$a_i' = a_i - \sum_{k=1}^{i-1} (q_k^{Tr} a_i) q_k$$

$$q_i = \frac{a_i'}{\|a_i'\|}$$

- Ortogonalna macierz Q

$$Q = [q_1 \ q_2 \ \ldots \ q_n]$$

- Macierz trójkątna górna R

$$r_{ii} = \|a_i'\|, \ i = 1, \ldots, n$$
$$r_{ij} = q_i^{Tr} a_j, \ i < j$$
$$r_{ij} = 0, \ i > j$$

[1]Np. nie nadaje się dla macierzy osobliwych, czyli mających przynajmniej jedną wartość własną równą zero; ale są też inne problemy