Eigen Vector Calculation

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I. Introduction

Eigenvalues play a fundamental role in linear algebra and have applications in physics, engineering, and data science. The QR algorithm is a widely used numerical method to compute eigenvalues. The algorithm relies on the QR decomposition of a matrix, which can be efficiently computed using the Gram-Schmidt process.

II. Gram-Schmidt Process

The Gram-Schmidt process transforms a set of linearly independent vectors into an orthonormal set of vectors. Given a set of vectors $\{\mathbf{a_1}, \mathbf{a_2}, \dots, \mathbf{a_n}\}$, it generates an orthonormal basis $\{\mathbf{q_1}, \mathbf{q_2}, \dots, \mathbf{q_n}\}$ satisfying:

$$\mathbf{q_i}^T \mathbf{q_j} = \begin{cases} 1 & \text{if } i = j, \\ 0 & \text{if } i \neq j. \end{cases}$$

A. Steps

1. Normalize $\mathbf{a_1}$ to get $\mathbf{q_1}$:

$$\mathbf{q_1} = \frac{\mathbf{a_1}}{\|\mathbf{a_1}\|}.$$

2. For each a_i, subtract its projections onto all previous q_j:

$$\mathbf{a_i'} = \mathbf{a_i} - \sum_{j=1}^{i-1} (\mathbf{q_j}^T \mathbf{a_i}) \mathbf{q_j}.$$

- Normalize a_i' to get q_i:

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

The Gram-Schmidt process ensures that $\mathbf{q_1}, \mathbf{q_2}, \dots, \mathbf{q_n}$ are orthonormal, forming the columns of the matrix $\mathbf{Q}$. This process is fundamental to QR decomposition. 3. The columns of $\mathbf{Q}$ are the orthonormal vectors $\mathbf{q_1}, \mathbf{q_2}, \dots, \mathbf{q_n}$.

4. The matrix $\mathbf{R}$ is an upper triangular matrix whose elements are the coefficients of the projections:

$$\mathbf{R}[i, j] = \mathbf{q_i}^T \mathbf{a_j} \quad \text{for } i \leq j.$$

This means each entry $\mathbf{R}[i, j]$ corresponds to the inner product of $\mathbf{q_i}$ and the column $\mathbf{a_j}$ from the original matrix.

Thus, the QR decomposition gives us two matrices:

$$\mathbf{A} = \mathbf{QR},$$

where $\mathbf{Q}$ is orthogonal, and $\mathbf{R}$ is upper triangular. where $\mathbf{Q}$ is orthogonal, and $\mathbf{R}$ is upper triangular.

III. QR Decomposition

A. Definition

QR decomposition factors a square matrix $\mathbf{A}$ into:

$$\mathbf{A} = \mathbf{QR},$$

where:

- $\mathbf{Q}$ is an orthogonal matrix whose columns are the orthonormal basis vectors computed using Gram-Schmidt.
- $\mathbf{R}$ is an upper triangular matrix containing the coefficients from the projections.

IV. Eigenvalue Computation Using QR Algorithm

A. Overview

The QR algorithm iteratively transforms a matrix into a nearly diagonal form. The eigenvalues appear on the diagonal of the transformed matrix after convergence.

B. Algorithm Steps

1) Input a square matrix $\mathbf{A}$.
2) Perform QR decomposition on $\mathbf{A}$ to obtain $\mathbf{Q}$ and $\mathbf{R}$ using Gram-Schmidt Process.
3) Iteratively update the matrix $\mathbf{A}$ to
$$\mathbf{A} = \mathbf{RQ}.$$
4) Stop when the off-diagonal sum of $\mathbf{A}$ is veru negligible or tolerance threshold.
5) After convergence, the diagonal entries of $\mathbf{A}$ are the eigenvalues.

C. Convergence Criterion

The iteration stops when the sum of the magnitudes of off-diagonal elements becomes smaller than a predefined tolerance. Mathematically:

$$\text{Off-diagonal sum} = \sum_{i \neq j} |\mathbf{A}[i, j]| < \text{tolerance}.$$

V. Convergence Criteria in the QR Algorithm

The convergence criteria in the QR algorithm ensures that the iterative process stops when the matrix is sufficiently close to a diagonal matrix. The diagonal elements of the matrix then represent the eigenvalues. The convergence is monitored by observing the magnitude of the off-diagonal elements in the matrix.

A. Tolerance Threshold

The tolerance is a small positive value that determines when the off-diagonal sum is small enough to stop the algorithm. A typical value for tolerance could be 10^{-12} or 10^{-15}, depending on the required accuracy.
If the sum of the off-diagonal elements falls below this threshold, the algorithm is considered to have converged. At this point, the matrix is nearly diagonal, and the diagonal entries represent the eigenvalues.

B. Mathematical Expression for Convergence

The QR algorithm stops when:

$$\sum_{i \neq j} |\mathbf{A}[i, j]| < \text{tolerance}.$$

This means that if the sum of the absolute values of the off-diagonal elements is smaller than the specified tolerance, the algorithm halts and the eigenvalues are taken as the diagonal elements of $\mathbf{A}$.

C. Practical Considerations

The algorithm's convergence can be affected by numerical errors, especially in cases of ill-conditioned matrices. In such cases, additional techniques like shifts may be applied to accelerate convergence.
The QR algorithm converges faster for matrices with well-separated eigenvalues. For matrices with close eigenvalues or poor conditioning, the algorithm may require more iterations to converge.

VI. Applications

The QR algorithm is commonly used in:

- Numerical solutions to eigenvalue problems.
- Principal Component Analysis (PCA) in data science.
- Vibrational analysis in mechanical systems.

VII. Conclusion

The QR decomposition and Gram-Schmidt process provide a systematic approach for numerical eigenvalue computation. While simple to understand and implement, these methods are computationally expensive for large matrices. Optimized numerical libraries are often preferred for practical applications.

1) Code to find Eigen Values

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code/eigen.py
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