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SS ZC416 Mathematical Foundations for Data Science
Singular Value Decomposition

Recap

- Gauss Jacobi Iterative Method
- Gauss Siedel Iterative Method

Orthogonal Matrix

A nxn matrix is orthogonal iff $A A^T = A^T A = I$

- All columns are pairwise orthogonal
- The determinant of an orthogonal matrix is +1 or –1

Example 1:

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

- A is an orthogonal matrix
- The columns are pairwise ~~orthogonal~~ orthonormal (Orthogonal + Unit Vectors)

  For example, $C_1 \times C_1^T = 1$ & $C_1 \times C_2^T = 0$

Diagonalization of Some Matrices

An nxn **matrix** is **diagonalizable** iff it admits n linearly independent eigenvectors

Suppose A is an nxn matrix with n linearly independent eigenvectors: $v_1, v_2, \ldots, v_n$

Let X = $[v_1, v_2, \ldots, v_n]$ be the matrix formed by the n eigenvectors.

X is an nxn matrix and is invertible (why?)

And $X A X^{-1} = D$, where D is the diagonal matrix formed by the eigenvalues of A

Example 2: Diagonalization of a Matrix

Consider the matrix $A = \begin{bmatrix} 1 & -3 & 3 \\ 3 & -5 & 3 \\ 6 & -6 & 4 \end{bmatrix}$

- The eigenvalue of A: λ = -2, -2, 4
- The eigenvectors: **λ = -2**: $\begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix}$ & **λ = 4**: $\begin{bmatrix} 1 \\ 1 \\ 2 \end{bmatrix}$
- These eigenvectors are linearly independent – There are 3 for the 3x3 matrix A
- Consider X, the matrix formed by the eigenvectors of A: $X = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 0 & 1 \\ 0 & -1 & 2 \end{bmatrix}$
- $X^{-1} = \begin{bmatrix} -0.5 & 1.5 & -0.5 \\ 1 & -1 & 0 \\ 0.5 & -0.5 & 0.5 \end{bmatrix}$
- $X^{-1}AX = \begin{bmatrix} -2 & 0 & 0 \\ 0 & -2 & 0 \\ 0 & 0 & 4 \end{bmatrix}$

Symmetric Matrices - Eigenvectors

Consider the matrix $A = \begin{bmatrix} 3 & 2 & 4 \\ 2 & 0 & 2 \\ 4 & 2 & 3 \end{bmatrix}$

- The eigenvalue of A: λ = -1, -1, 8 & The eigenvectors: **λ = -1**: $\begin{bmatrix} 1 \\ -2 \\ 0 \end{bmatrix}, \begin{bmatrix} 4 \\ 2 \\ -5 \end{bmatrix}$ & **λ = 8**: $\begin{bmatrix} 2 \\ 1 \\ 2 \end{bmatrix}$
- These eigenvectors are linearly independent and mutually orthogonal
- Consider X, the matrix formed by the eigenvectors of A: $X = \begin{bmatrix} 2/3 & 1/\sqrt{5} & 4/\sqrt{45} \\ 1/3 & -2/\sqrt{5} & 2/\sqrt{45} \\ 2/3 & 0 & -5/\sqrt{45} \end{bmatrix}$
- X is an orthonormal matrix
- $X^{-1}AX = \begin{bmatrix} 8 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$

Symmetric Matrix: X can be chosen to be a orthonormal matrix

Symmetric Matrices

1. We are given a dataset: $m = 100$ humans and $n = 1000$ gene expressions
2. The dataset is the $m \times n$ matrix A
3. Then $C = A^T A$

   C is a 1000×1000 symmetric matrix

4. We know that any matrix, and in particular A, can be expressed as $A = U \Sigma V^T$
5. Apply SVD to $Y = 1/\sqrt{n}\, A$

   Obtain $Y = USV^T$
6. Columns of U are eigenvectors of C

Singular Value Decomposition – SVD

1. Consider an m x n matrix A

2. It can be shown that any matrix, and therefore A, can be expressed as $A = U\Sigma V^T$

   Σ: A diagonal matrix; The diagonal entries σ_i are known as singular values of A

   U: An orthogonal matrix; The columns are known as the left-singular vectors of A

   V: An orthogonal matrix; The columns are known as the right-singular vectors of A

3. Then $Ax = U\Sigma V^T x$ may be considered as

   A Rotation followed by a Stretch followed by a Rotation

Application – PCA

1. We are given a dataset: m = 100 humans and n = 1000 gene expressions
2. The dataset is the m x n matrix A
3. Consider $C = A^TA$

   C is a 1000 x 1000 symmetric matrix
4. We know that any matrix, and in particular A, can be expressed as $A = U\Sigma V^T$

   Σ: A diagonal matrix; U: An orthogonal matrix; V: An orthogonal matrix

Now consider $C = A^TA = (V\Sigma^TU^T)*(U\Sigma V^T) = V\Sigma^T\Sigma V^T$

Therefore V must be the eigenvectors of C and Σ is diagonal with entries $\sqrt{\lambda}$'s

Thank you!!