LINEAR ALGEBRA FOR DATA SCIENCE

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DS3
Data Science Summer School

Hertie School
Data Science Lab

Lecturer

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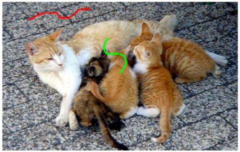
- PhD Candidate in Mathematics at TU Berlin
- Scientific Assistant at Zuse Institute Berlin
- Passionate about Artificial Intelligence
- I love to travel and lift weights

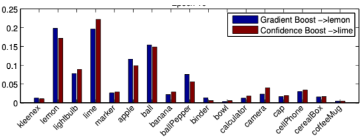
Why Data Science?

Typical problems in Data Science

- Image Segmentation

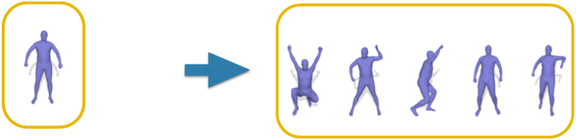


- Object Classifcation

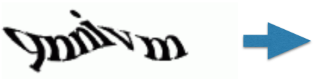


Typical problems in Data Science

- 3D Shape Analysis, e.g. Shape Retrieval



- Optical Character Recognition



“qnnivm”

Web, ads and recommendations

Google AdSense

Prerequisites for Data Science

Mathematical background in

- Linear Algebra (Today)
- Calculus (August 17)
- Statistics and Probability Theory (August 18)

Outline

Why Linear Algebra?

- Linear Algebra to compactly represent and operate on sets of linear equations
- E.g., system of equations

$$4x_1 - 5x_2 = -13$$
$$-2x_1 + 3x_2 = 9$$

- Matrix notation

$$Ax = b$$

with

$$A = \begin{bmatrix} 4 & -5 \\ -2 & 3 \end{bmatrix}, \quad b = \begin{bmatrix} -13 \\ 9 \end{bmatrix}$$

Basic Concepts and Notation

- $A \in \mathbb{R}^{m \times n}$ a matrix with m rows and n columns
- $x \in \mathbb{R}^n$ a vector of n entries
  $\hookrightarrow$ ***column vector*** - matrix with n rows and 1 column
  $\hookrightarrow$ ***row vector*** x^T
- i^{th} element of x is x_i

$$x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

- Purpose of vector is to visually represent a piece of data

Matrix Elements

- Entry of A in i^{th} row and j^{th} column is a_{ij} (or $A_{ij}, A_{i,j}$)

$$A = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \dots & a_{mn} \end{bmatrix}$$

- j^{th} column of A is a_j or $A_{:,j}$

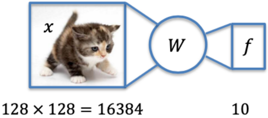
$$A = \begin{bmatrix} | & | & & | \\ a_1 & a_2 & \dots & a_n \\ | & | & & | \end{bmatrix}$$

- i^{th} row of A is a_i^T or $A_{i,:}$

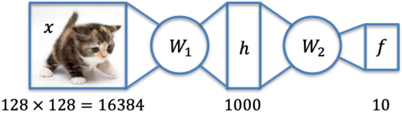
$$A = \begin{bmatrix} — & a_1^T & — \\ — & a_2^T & — \\ & \vdots & \\ — & a_n^T & — \end{bmatrix}$$

Application: Machine Learning

1−layer network $f = Wx$



2−layer network $f = W_2 \max(0, W_1 x)$



Matrix Multiplication

- Product of two matrices $A \in \mathbb{R}^{m \times n}$ and $B \in \mathbb{R}^{n \times p}$ is the matrix

$$C = AB \in \mathbb{R}^{m \times p}$$

where

$$C_{ij} = \sum_{k=1}^{n} A_{ik} B_{kj}$$

Vector-Vector Products

- ***Inner (dot) product*** of two vectors $x, y \in \mathbb{R}^n$ is a real number given by

$$x^T y \in \mathbb{R} = \begin{bmatrix} x_1 & x_2 & \dots & x_n \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = \sum_{i=1}^{n} x_i y_i$$

$\hookrightarrow$ special case of matrix multiplication
$\hookrightarrow$ note $x^T y = y^T x$

- ***Outer product*** of two vectors $x \in \mathbb{R}^m, y \in \mathbb{R}^n$ is a matrix whose entries are given by $(xy^T)_{ij} = x_i y_j$

$$xy^T \in \mathbb{R}^{m \times n} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \end{bmatrix} \begin{bmatrix} y_1 & y_2 & \dots & y_n \end{bmatrix} = \begin{bmatrix} x_1 y_1 & x_1 y_2 & \dots & x_1 y_n \\ x_2 y_1 & x_2 y_2 & \dots & x_2 y_n \\ \vdots & \vdots & \ddots & \vdots \\ x_m y_1 & x_m y_2 & \dots & x_m y_n \end{bmatrix}$$

Matrix-Vector Products

- Product of a matrix $A \in \mathbb{R}^{m \times n}$ and a vector $x \in \mathbb{R}^n$ is a vector $y = Ax \in \mathbb{R}^m$
  - If we write A by rows

$$y = Ax = \begin{bmatrix} — & a_1^T & — \\ — & a_2^T & — \\ & \vdots & \\ — & a_m^T & — \end{bmatrix} x = \begin{bmatrix} a_1^T x \\ a_2^T x \\ \vdots \\ a_m^T x \end{bmatrix}$$

  - If we write A by columns

$$y = Ax = \begin{bmatrix} | & | & & | \\ a_1 & a_2 & \cdots & a_n \\ | & | & & | \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} a_1 \end{bmatrix} x_1 + \begin{bmatrix} a_2 \end{bmatrix} x_2 + \cdots + \begin{bmatrix} a_n \end{bmatrix} x_n$$

$\hookrightarrow$ y is a ***linear combination*** of the columns of A

Matrix-Matrix Products

- Matrix-matrix as a set of vector-vector products

$$C = AB = \begin{bmatrix} — & a_1^T & — \\ — & a_2^T & — \\ & \vdots & \\ — & a_m^T & — \end{bmatrix} \begin{bmatrix} | & | & & | \\ b_1 & b_2 & \cdots & b_p \\ | & | & & | \end{bmatrix} = \begin{bmatrix} a_1^T b_1 & a_1^T b_2 & \cdots & a_1^T b_p \\ a_2^T b_1 & a_2^T b_2 & \cdots & a_2^T b_p \\ \vdots & \vdots & \ddots & \vdots \\ a_m^T b_1 & a_m^T b_2 & \cdots & a_m^T b_p \end{bmatrix}$$

$\hookrightarrow$ $(i,j)^{th}$ entry of C equals inner product of i^{th} row of A and j^{th} column of B

- Represent A by columns, B by rows

$$C = AB = \begin{bmatrix} | & | & & | \\ a_1 & a_2 & \cdots & a_n \\ | & | & & | \end{bmatrix} \begin{bmatrix} — & b_1^T & — \\ — & b_2^T & — \\ & \vdots & \\ — & b_n^T & — \end{bmatrix} = \sum_{i=1}^{n} a_i b_i^T$$

$\hookrightarrow$ AB is equal to the sum, over all i, of the outer product of the i^{th} column of A and i^{th} row of B

Matrix-Matrix Products

- Matrix-matrix multiplication as a set of matrix-vector products

$$C = AB = A \begin{bmatrix} | & | & & | \\ b_1 & b_2 & \cdots & b_p \\ | & | & & | \end{bmatrix} = \begin{bmatrix} | & | & & | \\ Ab_1 & Ab_2 & \cdots & Ab_p \\ | & | & & | \end{bmatrix}$$

$\hookrightarrow$ i^{th} column of C is given by the matrix-vector product with the vector on the right, $c_i = Ab_i$

- Represent A by rows, view rows of C as matrix-vector product between rows of A and C

$$C = AB = \begin{bmatrix} — & a_1^T & — \\ — & a_2^T & — \\ & \vdots & \\ — & a_m^T & — \end{bmatrix} B = \begin{bmatrix} — & a_1^T B & — \\ — & a_2^T B & — \\ & \vdots & \\ — & a_m^T B & — \end{bmatrix}$$

$\hookrightarrow$ i^{th} row of C is given by the matrix-vector product with the vector on the left, $c_i^T = a_i^T B$

Matrix multiplication properties

- Matrix multiplication is associative

$$(AB)C = A(BC)$$

Proof

$$\begin{aligned}
((AB)C)_{ij} &= \sum_{k=1}^{p} (AB)_{ik} C_{kj} = \sum_{k=1}^{p} \left(\sum_{l=1}^{n} A_{il} B_{lk} \right) C_{kj} \\
&= \sum_{k=1}^{p} \left(\sum_{l=1}^{n} A_{il} B_{lk} C_{kj} \right) = \sum_{l=1}^{n} \left(\sum_{k=1}^{p} A_{il} B_{lk} C_{kj} \right) \\
&= \sum_{l=1}^{n} A_{il} \left(\sum_{k=1}^{p} B_{lk} C_{kj} \right) = \sum_{l=1}^{n} A_{il} (BC)_{lj} = (A(BC))_{ij}
\end{aligned}$$

- Matrix multiplication is distributive

$$A(B + C) = AB + AC$$

- Matrix multiplication is, in general, not commutative $AB \neq BA$
  $\hookrightarrow$ If $A \in \mathbb{R}^{m \times n}$, $B \in \mathbb{R}^{n \times q}$, then BA does not exist if m and q are not equal !

Identity Matrix and Diagonal Matrices

- ***Identity matrix*** $I \in \mathbb{R}^{n \times n}$ defined as

$$I_{ij} = \begin{cases} 1, & i = j \\ 0, & i \neq j \end{cases}$$

- $AI = A = IA$

- ***Diagonal matrix*** $D = \text{diag}(d_1, d_2, ..., d_n)$

$$D_{ij} = \begin{cases} d_i, & i = j \\ 0, & i \neq j \end{cases}$$

- $I = \text{diag}(1, 1, ..., 1)$

The Transpose

- ***Transpose*** of a matrix $A \in \mathbb{R}^{m \times n}$ is $A^T \in \mathbb{R}^{n \times m}$ where

$$(A^T)_{ij} = A_{ji}$$

Properties

- $(A^T)^T = A$
- $(AB)^T = B^T A^T$
- $(A + B)^T = A^T + B^T$

Symmetric Matrices

- $A \in \mathbb{R}^{n \times n}$ is ***symmetric*** if $A = A^T$
- $A \in \mathbb{R}^{n \times n}$ is ***anti-symmetric*** if $A = -A^T$

Properties

- $A + A^T$ is symmetric, $A - A^T$ is anti-symmetric
- $A = \frac{1}{2}(A + A^T) + \frac{1}{2}(A - A^T)$
- $\mathbb{S}^n$ - set of symmetric matrices of size n

The Trace

- ***Trace*** of $A \in \mathbb{R}^{n \times n}$

$$\operatorname{tr} A = \sum_{i=1}^{n} A_{ii}$$

Properties

- $A \in \mathbb{R}^{n \times n}, \operatorname{tr} A = \operatorname{tr} A^T$
- $A, B \in \mathbb{R}^{n \times n}, \operatorname{tr}(A + B) = \operatorname{tr} A + \operatorname{tr} B$
- $A \in \mathbb{R}^{n \times n}, t \in \mathbb{R}, \operatorname{tr}(tA) = t \operatorname{tr} A$
- A, B such that AB is square, $\operatorname{tr} AB = \operatorname{tr} BA$

Proof

$$\begin{aligned}
\operatorname{tr} AB &= \sum_{i=1}^{m} (AB)_{ii} = \sum_{i=1}^{m} \left(\sum_{j=1}^{n} A_{ij} B_{ji} \right) \\
&= \sum_{i=1}^{m} \sum_{j=1}^{n} A_{ij} B_{ji} = \sum_{j=1}^{n} \sum_{i=1}^{m} B_{ji} A_{ij} \\
&= \sum_{j=1}^{n} \left(\sum_{i=1}^{m} B_{ji} A_{ij} \right) = \sum_{j=1}^{n} (BA)_{jj} = \operatorname{tr} BA
\end{aligned}$$

- A, B, C such that ABC is square, $\operatorname{tr} ABC = \operatorname{tr} BCA = \operatorname{tr} CAB$

Norms

- ***Norm*** is any function $f : \mathbb{R}^n \to \mathbb{R}$ satisfying
  1. $\forall x \in \mathbb{R}^n, f(x) \geq 0$ (non-negativity)
  2. $f(x) = 0$ if and only if $x = 0$ (definiteness)
  3. $x \in \mathbb{R}^n, t \in \mathbb{R}, f(tx) = |t| f(x)$ (homogeneity)
  4. $\forall x, y \in \mathbb{R}^n, f(x + y) \leq f(x) + f(y)$ (triangle inequality)

- ℓ_p norm $\|x\|_p = \left(\sum_{i=1}^n |x_i|^p\right)^{1/p}$
  - ℓ_2 (Euclidean) norm measures the 'length' of the vector

$$\|x\|_2 = \sqrt{\sum_{i=1}^n x_i^2}$$

  - ℓ_1 norm

$$\|x\|_1 = \sum_{i=1}^n |x_i|$$

  - ℓ_∞ norm

$$\|x\|_\infty = \max_i |x_i|$$

- Frobenius norm $\|A\|_F = \sqrt{\sum_{i=1}^m \sum_{j=1}^n A_{ij}^2} = \sqrt{\mathrm{tr}(A^T A)}$

Norm Exercise

Exercise

Show that the length of Ax equals the length of $A^T x$ if $AA^T = A^T A$.

Solution

$$\begin{aligned}
\|Ax\|^2 &= (Ax)^T (Ax) \\
&= x^T A^T A x \\
&= x^T A A^T x \\
&= (A^T x)^T (A^T x) \\
&= \|A^T x\|^2
\end{aligned}$$

Norm Exercise

Exercise

Show that the length of Ax equals the length of $A^T x$ if $AA^T = A^T A$.

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&= x^T A A^T x \\
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&= \|A^T x\|^2
\end{aligned}$$

Linear (In)dependence

- Set $\{x_1, x_2, ..., x_n\} \subset \mathbb{R}^m$ is ***(linearly) independent*** if no vector can be represented as linear combination of remaining vectors
- Set $\{x_1, x_2, ..., x_n\} \subset \mathbb{R}^m$ is ***(linearly) dependent*** if one vector can be represented as a linear combination of the remaining vectors

$$x_n = \sum_{i=1}^{n-1} \alpha_i x_i, \quad \alpha_1, ..., \alpha_{n-1} \in \mathbb{R}$$

- E.g. $x_1 = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}, \quad x_1 = \begin{bmatrix} 4 \\ 1 \\ 5 \end{bmatrix}, \quad \mathrm{x}_1 = \begin{bmatrix} 2 \\ -3 \\ -1 \end{bmatrix}$ linearly dependent $(x_3 = -2x_1 + x_2)$

Rank

- ***Column rank*** of $A \in \mathbb{R}^{m \times n}$ is the size of largest subset of columns of A that consitute a linearly independent set
- ***Row rank*** of $A \in \mathbb{R}^{m \times n}$ is the size of largest subset of rows of A that consitute a linearly independent set
- For any $A \in \mathbb{R}^{m \times n}$ the column rank of A equals the row rank of A - $\boldsymbol{rank}(A)$

Properties

- For $A \in \mathbb{R}^{m \times n}, \operatorname{rank}(A) \leq \min(m, n)$
- A is ***full rank*** if $\operatorname{rank}(A) = \min(m, n)$
- $A \in \mathbb{R}^{m \times n}, \operatorname{rank}(A) = \operatorname{rank}(A^T)$
- $A \in \mathbb{R}^{m \times n}, B \in \mathbb{R}^{n \times p}, \operatorname{rank}(AB) \leq \min(\operatorname{rank}(A), \operatorname{rank}(B))$
- $A, B \in \mathbb{R}^{m \times n}, \operatorname{rank}(A + B) \leq \operatorname{rank}(A) + \operatorname{rank}(B)$

The Inverse

- ***Inverse*** of $A \in \mathbb{R}^{n \times n}$, A^{-1}, is the unique matrix

$$A^{-1}A = I = AA^{-1}$$

- Note not all matrices have inverses (e.g., non-square matrices)
- A is ***invertible (non-singular)*** if A^{-1} exists and ***non-invertible (singular)*** otherwise
- A has an inverse A^{-1} if A is of full rank

Properties for $A, B \in \mathbb{R}^{n \times n}$
- $(A^{-1})^{-1} = A$
- $(AB)^{-1} = B^{-1}A^{-1}$
- $(A^{-1})^T = (A^T)^{-1}$, often denoted by A^{-T}

Inverse Usage

Consider $Ax = b$ where $A \in \mathbb{R}^{n \times n}$ and $x, b \in \mathbb{R}^n$. If A is non-singular (invertible), then $x = A^{-1}b$

- What if $A \in \mathbb{R}^{m \times n}$ is not a square matrix ?

The Determinant

- ***Determinant*** of $A \in \mathbb{R}^{n\times n}$, $|A|$ or $\det A$, is a function $\det : \mathbb{R}^{n\times n} \to \mathbb{R}$
- $A_{\setminus i,\setminus j} \in \mathbb{R}^{(n-1)\times(n-1)}$ is the matrix resulting from deleting i^{th} row and j^{th} column from A
- Recursive formula

$$
\begin{aligned}
|A| &= \sum_{i=1}^{n} (-1)^{i+j} a_{ij} |A_{\setminus i,\setminus j}| \quad \text{for any } j \in 1, ..., n \\
&= \sum_{j=1}^{n} (-1)^{i+j} a_{ij} |A_{\setminus i,\setminus j}| \quad \text{for any } i \in 1, ..., n
\end{aligned}
$$

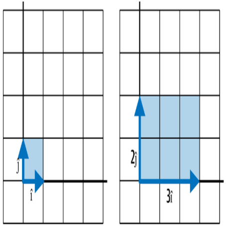
with initial $|A| = a_{11}$ for $A \in \mathbb{R}^{1\times 1}$

  - $\left| \begin{bmatrix} a_{11} \end{bmatrix} \right| = a_{11}$
  - $\left| \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \right| = a_{11}a_{22} - a_{12}a_{21}$
  - $\left| \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \right| = a_{11} \left| \begin{bmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{bmatrix} \right| - a_{12} \left| \begin{bmatrix} a_{21} & a_{23} \\ a_{31} & a_{33} \end{bmatrix} \right| + a_{13} \left| \begin{bmatrix} a_{21} & a_{22} \\ a_{31} & a_{32} \end{bmatrix} \right|$

Determinant Properties

- $|I| = 1$
- $$\left|\begin{bmatrix} — & ta_1^T & — \\ — & a_2^T & — \\ & \vdots & \\ — & a_m^T & — \end{bmatrix}\right| = t|A|$$
- $$\left|\begin{bmatrix} — & a_2^T & — \\ — & a_1^T & — \\ & \vdots & \\ — & a_m^T & — \end{bmatrix}\right| = -|A|$$

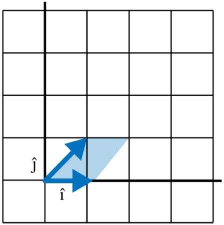
- Describes how much a sampled area changes in scale with linear transformations



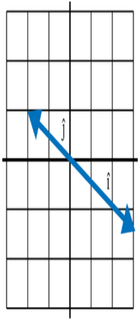
- $A \in \mathbb{R}^{n\times n}, |A| = |A^T|$
- $A, B \in \mathbb{R}^{n\times n}, |AB| = |A||B|$
- $A \in \mathbb{R}^{n\times n}, |A| = 0$ if and only if A is singular (non-invertible)
- $A \in \mathbb{R}^{n\times n}$ and A non-singular, $|A^{-1}| = 1/|A|$

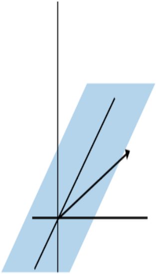
Determinant Properties

- Shears and rotations do not affect determinant



- Linearly dependent transformations result in determinant 0
  - In $2D$ space is compressed into one dimension
  - In $3D$ space is compressed into two dimensions





Determinant Exercise

Exercise

If $A \in \mathbb{R}^{n \times n}$ has determinant $\frac{1}{2}$, find $|2A|, |-A|, |A^2|, |A^{-1}|$

Solution

- $|2A| = 2^n|A| = 2^{n-1}$
- $|-A| = (-1)^n|A| = (-1)^n/2$
- $|A^2| = |A||A| = 1/4$
- $|A^{-1}| = \frac{1}{|A|} = 2$ (as $|A| \neq 0$)

Determinant Exercise

Exercise

If $A \in \mathbb{R}^{n \times n}$ has determinant $\frac{1}{2}$, find $|2A|, |-A|, |A^2|, |A^{-1}|$

Solution

- $|2A| = 2^n|A| = 2^{n-1}$
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- $|A^2| = |A||A| = 1/4$
- $|A^{-1}| = \frac{1}{|A|} = 2$ (as $|A| \neq 0$)

Determinant Exercise

Exercise

Find the determinants of

$$A = \begin{bmatrix} 1 \\ 4 \\ 2 \end{bmatrix} \begin{bmatrix} 2 & -1 & 2 \end{bmatrix}, \quad U = \begin{bmatrix} 4 & 4 & 8 & 8 \\ 0 & 1 & 2 & 2 \\ 0 & 0 & 2 & 6 \\ 0 & 0 & 0 & 2 \end{bmatrix}, \quad \mathrm{U}^T \text{ and } \mathrm{U}^{-1}$$

Solution

- $|A| = \left| \begin{bmatrix} 1 \\ 4 \\ 2 \end{bmatrix} \begin{bmatrix} 2 & -1 & 2 \end{bmatrix} \right| = \left| \begin{bmatrix} 2 & -1 & 2 \\ 8 & -4 & 8 \\ 4 & -2 & 4 \end{bmatrix} \right| = 2(-16+16)+1(32-32)+2(-16+16) = 0$
- $|U| = 4 \times 1 \times 2 \times 2 = 16 = |U^T|, \quad$ as U is an upper diagonal matrix
- $U^{-1} = \frac{1}{|U|} = \frac{1}{16}$

Determinant Exercise

Exercise

Find the determinants of

$$A = \begin{bmatrix} 1 \\ 4 \\ 2 \end{bmatrix} \begin{bmatrix} 2 & -1 & 2 \end{bmatrix}, \quad U = \begin{bmatrix} 4 & 4 & 8 & 8 \\ 0 & 1 & 2 & 2 \\ 0 & 0 & 2 & 6 \\ 0 & 0 & 0 & 2 \end{bmatrix}, \quad \mathrm{U}^T \text{ and } \mathrm{U}^{-1}$$

Solution

- $|A| = \left| \begin{bmatrix} 1 \\ 4 \\ 2 \end{bmatrix} \begin{bmatrix} 2 & -1 & 2 \end{bmatrix} \right| = \left| \begin{bmatrix} 2 & -1 & 2 \\ 8 & -4 & 8 \\ 4 & -2 & 4 \end{bmatrix} \right| = 2(-16+16)+1(32-32)+2(-16+16) = 0$
- $|U| = 4 \times 1 \times 2 \times 2 = 16 = |U^T|,$ as U is an upper diagonal matrix
- $U^{-1} = \frac{1}{|U|} = \frac{1}{16}$

Eigenvalues and Eigenvectors

- $\lambda \in \mathbb{C}$ is an ***eigenvalue*** and $x \in \mathbb{C}^n$ is the corresponding ***eigenvector*** of $A \in \mathbb{R}^{n \times n}$ if

$$Ax = \lambda x, \quad x \neq 0$$

- (λ, x) is an eigenvalue-eigenvector pair of A if

$$(\lambda I - A)x = 0, \quad x \neq 0$$

- Equation has a non-zero solution to x if and only if $(\lambda I - A)$ is singular

$$|(\lambda I - A)| = 0$$

- Polynomial in λ of order n

$$p(\lambda_i) = \lambda_i^n + c_{n-1}\lambda_i^{n-1} + ... + c_1\lambda_i + c_0$$

- Roots of ***characteristic polynomial*** $\lambda_1, \lambda_2, ..., \lambda_n$ are the eigenvalues of A
- Eigenvector corresponding to eigenvalue λ_i

$$(\lambda_i I - A)x = 0$$

Properties of Eigenvalues and Eigenvectors

- For any eigenvector $x \in \mathbb{C}^n$ and a scalar $t \in \mathbb{C}$, $A(cx) = cAx = x\lambda x = \lambda(cx)$, so cx is also an eigenvector
- The eigenvector associated with λ is normalized to have length 1

- $\operatorname{tr} A = \sum_{i=1}^{n} \lambda_i$
- $|A| = \prod_{i=1}^{n} \lambda_i$
- Rank of A equals the number of non-zero eigenvalues of A
- If A non-singular then $1/\lambda_i$ is an eigenvalue of A^{-1} with associated eigenvector x_i

$$A^{-1}x_i = (1/\lambda_i)x_i$$

- Eigenvalues of diagonal matrix $D = \operatorname{diag}(d_1, ..., d_n)$ are the diagonal entries $d_1, ..., d_n$

Eigendecomposition

- Write eigenvector equations simultaneously

$$AX = X\Lambda$$

- Columns of $X \in \mathbb{R}^{n\times n}$ are eigenvectors of A
- Λ is a diagonal matrix whose entries are eigenvalues of A

$$X \in \mathbb{R}^{n\times n} = \begin{bmatrix} | & | & & | \\ x_1 & x_2 & \cdots & x_n \\ | & | & & | \end{bmatrix}, \quad \Lambda = \mathrm{diag}(\lambda_1, ..., \lambda_n)$$

- If eigenvectors of A are linearly independent, then matrix X is invertible

$$A = X\Lambda X^{-1}$$

- A matrix written in such a form is ***diagonalizable***
- $A \in \mathbb{S}^n$
  - All eigenvalues of A are real
  - Eigenvectors of A are orthonormal (X is orthogonal, denoted by U)
  - $A = U\Lambda U^T$

Eigendecomposition Exercise

Exercise

Find eigenvalues and eigenvectors of $A = \begin{bmatrix} 3 & 4 & 2 \\ 0 & 1 & 2 \\ 0 & 0 & 0 \end{bmatrix}$ and $B = \begin{bmatrix} 0 & 0 & 2 \\ 0 & 2 & 0 \\ 2 & 0 & 0 \end{bmatrix}$, their traces and their determinants

Solution

- $|A| = 0$
- $\mathrm{tr}(A) = 4$
-

$$
\begin{aligned}
|A - \lambda I| &= 0 \\
\left| \begin{bmatrix} 3-\lambda & 4 & 2 \\ 0 & 1-\lambda & 2 \\ 0 & 0 & -\lambda \end{bmatrix} \right| &= 0 \\
(3-\lambda)(\lambda^2 - \lambda) &= 0
\end{aligned}
$$

Eigenvalues are $\lambda = \{0, 1, 3\}$ and their corresponding eigenvectors $\begin{bmatrix} 2 \\ -2 \\ 1 \end{bmatrix}, \begin{bmatrix} -2 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$

Eigendecomposition Exercise

Exercise

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Eigendecomposition Exercise

Solution

- $|B| = -8$ (recall product of eigenvalues)
- $\mathrm{tr}(B) = 2$ (recall sum of eigenvalues)
- $$\begin{aligned} |B - \lambda I| &= 0 \\ \left| \begin{bmatrix} -\lambda & 0 & 2 \\ 0 & 2-\lambda & 0 \\ 2 & 0 & -\lambda \end{bmatrix} \right| &= 0 \\ (-\lambda)(2-\lambda)(-\lambda) - 4(2-\lambda) &= 0 \\ (\lambda^2 - 4)(2-\lambda) = 0 \end{aligned}$$

  Eigenvalues are $\lambda = \{-2, 2, 2\}$
- To find eigenvectors

$$\begin{bmatrix} 0 & 0 & 2 \\ 0 & 2 & 0 \\ 2 & 0 & 0 \end{bmatrix} \begin{bmatrix} -1 \\ 0 \\ 1 \end{bmatrix} = -2 \begin{bmatrix} -1 \\ 0 \\ 1 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 2 \\ 0 & 2 & 0 \\ 2 & 0 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} = 2 \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 2 \\ 0 & 2 & 0 \\ 2 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} = 2 \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$$

- Note the relations are also valid for normalized eigenvectors

Systems of Equations and Inverse Matrices

- Basic use of linear algebra is to solve systems of equations

$$\begin{aligned} 4x + 2y + 4z &= 44 \\ 5x + 3y + 7z &= 56 \\ 9x + 3y + 6z &= 72 \end{aligned}$$

Solutions

1. Solve it manually with algebraic operations to isolate three variables
2. Express the problem in terms of matrices and let a computer solve it

$$\text{Solve } AX = B \text{ where}$$

$$A = \begin{bmatrix} 4 & 2 & 4 \\ 5 & 3 & 7 \\ 9 & 3 & 6 \end{bmatrix}, \quad B = \begin{bmatrix} 44 \\ 56 \\ 72 \end{bmatrix}, \quad X = \begin{bmatrix} x \\ y \\ z \end{bmatrix}$$

1. Solve by hand using Gaussian elimination
2. Use a computer to find inverse matrix A^{-1}

Eigendecomposition Exercise

Exercise

Using the characteristic polynomial, find the relationship between trace, determinants and eigenvalues of any square matrix

Solution

- Let $A = \begin{bmatrix} a_{11} & \cdots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{n1} & \cdots & a_{nn} \end{bmatrix}$ whose eigenvalues are $\lambda_1, ..., \lambda_n$
- Characteristic polynomial $p(\lambda) = |\lambda I - A| = \lambda_n + c_{n-1}\lambda^{n-1} + \cdots + c_1\lambda + c_0$
- Also $p(\lambda) = (\lambda - \lambda_1)\cdots(\lambda - \lambda_n)$ (Eigenvalues of A are zeros of $p(\lambda)$)
- Express determinant as product of eigenvalues
  1. $p(0) = (0 - \lambda_1)\cdots(0 - \lambda_n) = (-1)^n \lambda_1 \cdots \lambda_n$
  2. $p(0) = |0I - A| = |-A| = (-1)^n |A|$

  $\hookrightarrow c_0 = (-1)^n \lambda_1 \cdots \lambda_n = (-1)^n |A| \implies |A| = \lambda_1 \cdots \lambda_n$

Eigendecomposition Exercise

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Using the characteristic polynomial, find the relationship between trace, determinants and eigenvalues of any square matrix

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  $\hookrightarrow c_0 = (-1)^n\lambda_1\cdots\lambda_n = (-1)^n|A| \implies |A| = \lambda_1\cdots\lambda_n$

Eigendecomposition Exercise

Solution

- Express trace as sum of eigenvalues
  1. Expand $p(\lambda) = (\lambda - \lambda_1)\cdots(\lambda - \lambda_n)$ to get λ^{n-1} term

$$-\lambda_1\lambda^{n-1} - \cdots - \lambda\lambda^{n-1} = -(\lambda_1 + \cdots + \lambda_n)\lambda^{n-1} \implies c_{n-1} = -(\lambda_1 + \cdots + \lambda_n)$$

  2. Expand $|\lambda I - A| = \left| \begin{bmatrix} \lambda - a_{11} & -a_{12} & \cdots & -a_{1n} \\ -a_{21} & \lambda - a_{22} & \cdots & -a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ -a_{n1} & -a_{n2} & \cdots & \lambda - a_{nn} \end{bmatrix} \right|$

     $\hookrightarrow p(\lambda) = (\lambda - a_{11})\cdots(\lambda - a_{nn}) + q(\lambda)$
     $\hookrightarrow q(\lambda)$ has degree at most $n-2$, hence no λ^{n-1} term
     $\hookrightarrow \lambda^{n-1}$ term must be from $(\lambda - a_{11})\cdots(\lambda - a_{nn})$
     $\hookrightarrow -(a_{11} + \cdots + a_{nn})\lambda^{n-1}$

$\hookrightarrow c_{n-1} = -(\lambda_1 + \lambda_n) = -(a_{11} + \cdots + a_{nn}) \implies \mathrm{tr}(A) = \lambda_1 + \cdots + \lambda_n$

Eigendecomposition Exercise

Exercise

Diagonalize unitary matrix $V = \frac{1}{\sqrt{3}}\begin{bmatrix} 1 & 1-i \\ 1+i & -1 \end{bmatrix}$ to reach $V = U\Lambda U^T$

Solution

$$\begin{aligned} |V - \lambda I| &= 0 \\ (1-\sqrt{3}\lambda)(-1-\sqrt{3}\lambda) - (1+i-i-i^2) &= 0 \\ 3\lambda^2 &= 3 \end{aligned}$$

- Eigenvalues are $\lambda = \{1, -1\}$, hence $\Lambda = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}$
- Corresponding eigenvectors $\begin{bmatrix} -0.366 + 0.366i \\ 1 \end{bmatrix}, \begin{bmatrix} 1.366 - 1.366i \\ 1 \end{bmatrix}$
- Normalize eigenvectors to get $U = \begin{bmatrix} \frac{-0.366+0.366i}{1.126} & \frac{1.366-1.366i}{2.175} \\ \frac{1}{1.126} & \frac{1}{2.175} \end{bmatrix}$

Eigendecomposition Exercise

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Eigendecomposition Exercise

Homework

Suppose T is a 3×3 upper triangular matrix with entries t_{ij}. Compare entries of $T^T T$ and TT^T. Show that if they are equal, then T must be diagonal.

Singular Value Decomposition (SVD)

- Generalization of eigendecomposition to $m \times n$ matrices
- $A = U\Lambda V^T$
  - U is $m \times m$ unitary matrix, whose column vectors are ***left-singular vectors***
  - Λ is $m \times n$ rectangular diagonal matrix, whose values σ_i are ***singular values***
  - V is $n \times n$ unitary matrix, whose column vectors are ***right-singular vectors***
- Singular values of $m \times n$ matrix A are equal to positive square roots of non-zero eignelvalues of $n \times n$ matrix $A^T A$ (and AA^T)
- Eigenvectors of AA^T are columns of U
- Eigenvectors of $A^T A$ are columns of V

SVD Exercise

Exercise

Find singular values and singular vectors of $A = \begin{bmatrix} 1 & 4 \\ 2 & 8 \end{bmatrix}$

Solution

- $A^T A = \begin{bmatrix} 1 & 2 \\ 4 & 8 \end{bmatrix} \begin{bmatrix} 1 & 4 \\ 2 & 8 \end{bmatrix} = \begin{bmatrix} 5 & 20 \\ 20 & 80 \end{bmatrix}$
  - $$\begin{aligned} \left| \begin{bmatrix} 5-\lambda & 20 \\ 20 & 80-\lambda \end{bmatrix} \right| &= 0 \\ (5-\lambda)(80-\lambda) - 400 &= 0 \end{aligned}$$

  $\hookrightarrow \lambda = \{0, 85\}$ hence singular values are $\{0, \sqrt{85}\}$ and eigenvectors $\begin{bmatrix} 1 \\ 4 \end{bmatrix}, \begin{bmatrix} -4 \\ 1 \end{bmatrix}$
- $AA^T = \begin{bmatrix} 1 & 4 \\ 2 & 8 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 4 & 8 \end{bmatrix} = \begin{bmatrix} 17 & 34 \\ 34 & 68 \end{bmatrix}$
  - Similarly for AA^T we have $\lambda = \{85, 0\}$ and eigenvectors $\begin{bmatrix} 1 \\ 2 \end{bmatrix}, \begin{bmatrix} -2 \\ 1 \end{bmatrix}$

$\hookrightarrow \Sigma = \begin{bmatrix} \sqrt{85} & 0 \\ 0 & 0 \end{bmatrix}, \quad U = \begin{bmatrix} \frac{1}{\sqrt{5}} & -\frac{2}{\sqrt{5}} \\ \frac{2}{\sqrt{5}} & \frac{1}{\sqrt{5}} \end{bmatrix}, \quad V = \begin{bmatrix} \frac{1}{\sqrt{17}} & -\frac{4}{\sqrt{17}} \\ \frac{4}{\sqrt{17}} & \frac{1}{\sqrt{17}} \end{bmatrix}$

SVD Exercise

Exercise

Explain how $U\Sigma V^T$ expresses A as a sum or r rank-1 matrices $A = \sigma_1 u_1 v_1^T + \cdots + \sigma_r u_r v_r^T$

Solution

- $A = U\Sigma V^T$
- $\epsilon_i = \text{diag}(0, ..., \sigma_i, ..., 0)$
- $\Sigma = \sum_i \epsilon_i$ and $\epsilon_i \neq 0$ if and only if $i \in \{1, \cdots, k\}$

$$
\begin{aligned}
A = U\Sigma V^T &= U(\Sigma_i \epsilon_i)V^T \\
&= \sum_{i=1}^{k} U\epsilon_i V^T
\end{aligned}
$$

SVD Exercise

Exercise

If A changes to $4A$ what is the change in SVD? What is the SVD for A^T and for A^{-1}?

Solution

- $4A = U(4\Sigma)V^T$, singular values of $4A$ are 4 times that of A
- $$\begin{aligned} A^T &= (U\Sigma V^T)^T \\ &= (V^T)^T \Sigma^T U^T \\ &= V\Sigma^T U^T \end{aligned}$$
- $$\begin{aligned} A^{-1} &= (U\Sigma V^T)^{-1} \\ &= (V^T)^{-1}\Sigma^{-1}U^{-1} \\ &= V\Sigma^{-1}U^T \end{aligned}$$
- $\Sigma^{-1} = \text{diag}(1/\sigma_1, \cdots, 1/\sigma_n)$
- U, V orthogonal $\implies UU^T = U^TU = I$ and $VV^T = V^TV = I$
- Double check $A^{-1}A = I$

SVD Exercise

Exercise

If A changes to $4A$ what is the change in SVD? What is the SVD for A^T and for A^{-1}?

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-
$$\begin{aligned} A^T &= (U\Sigma V^T)^T \\ &= (V^T)^T \Sigma^T U^T \\ &= V \Sigma^T U^T \end{aligned}$$
-
$$\begin{aligned} A^{-1} &= (U\Sigma V^T)^{-1} \\ &= (V^T)^{-1} \Sigma^{-1} U^{-1} \\ &= V \Sigma^{-1} U^T \end{aligned}$$
- $\Sigma^{-1} = \text{diag}(1/\sigma_1, \cdots, 1/\sigma_n)$
- U, V orthogonal $\Longrightarrow$ $UU^T = U^T U = I$ and $VV^T = V^T V = I$
- Double check $A^{-1}A = I$

Pseudoinverse

- Regression model in Machine Learning requires the computation of (Moore-Penrose) ***pseudoinverse***

$$A^\dagger = (U\Lambda V^T)^\dagger = VD^\dagger U^T$$

  - $D^\dagger$ is pseudo-inverse of D

$$\sigma_i^\dagger = \begin{cases} 1/\sigma_i, & \text{if } \sigma_i \neq 0 \\ 0, & otherwise \end{cases}$$

Pseudoinverse Exercise

Exercise

Find SVD and pseudoinverse of $A = \begin{bmatrix} 1 & 1 & 1 & 1 \end{bmatrix}$, $B = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}$, and $C = \begin{bmatrix} 1 & 1 \\ 0 & 0 \end{bmatrix}$

Solution

- $A^T A = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} \begin{bmatrix} 1 & 1 & 1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix}$
- $AA^T = \begin{bmatrix} 4 \end{bmatrix}$
- Solving $|A^T A - \lambda I| = 0$ and $|AA^T - \lambda I| = 0$ we find $\lambda = \{4, 0, 0, 0\}$
- Corresponding eigenvectors $\begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}, \begin{bmatrix} -1 \\ 0 \\ 0 \\ 1 \end{bmatrix}, \begin{bmatrix} -1 \\ 0 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} -1 \\ 1 \\ 0 \\ 0 \end{bmatrix}$

$\hookrightarrow \Sigma = \begin{bmatrix} 2 & 0 & 0 & 0 \end{bmatrix}, \quad U = \begin{bmatrix} 4 \end{bmatrix}, \quad V = \begin{bmatrix} \frac{1}{2} & -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{2} & 0 & 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{2} & 0 & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{2} & \frac{1}{\sqrt{2}} & 0 & 0 \end{bmatrix}$

Pseudoinverse Exercise

Exercise

Find SVD and pseudoinverse of $A = \begin{bmatrix} 1 & 1 & 1 & 1 \end{bmatrix}$, $B = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}$, and $C = \begin{bmatrix} 1 & 1 \\ 0 & 0 \end{bmatrix}$

Solution

- $A^T A = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} \begin{bmatrix} 1 & 1 & 1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix}$
- $AA^T = \begin{bmatrix} 4 \end{bmatrix}$
- Solving $|A^T A - \lambda I| = 0$ and $|AA^T - \lambda I| = 0$ we find $\lambda = \{4, 0, 0, 0\}$
- Corresponding eigenvectors $\begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}, \begin{bmatrix} -1 \\ 0 \\ 0 \\ 1 \end{bmatrix}, \begin{bmatrix} -1 \\ 0 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} -1 \\ 1 \\ 0 \\ 0 \end{bmatrix}$

$$\hookrightarrow \Sigma = \begin{bmatrix} 2 & 0 & 0 & 0 \end{bmatrix}, \quad U = \begin{bmatrix} 4 \end{bmatrix}, \quad V = \begin{bmatrix} \frac{1}{2} & -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{2} & 0 & 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{2} & 0 & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{2} & \frac{1}{\sqrt{2}} & 0 & 0 \end{bmatrix}$$

Pseudoinverse Exercise

Solution

- Pseudoinverse $A^\dagger = V\Sigma^\dagger U^T$
- $A^\dagger = \begin{bmatrix} \frac{1}{2} & -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{2} & 0 & 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{2} & 0 & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{2} & \frac{1}{\sqrt{2}} & 0 & 0 \end{bmatrix} \begin{bmatrix} \frac{1}{2} \\ 0 \\ 0 \\ 0 \end{bmatrix} [4] = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$
- $B^T B = \begin{bmatrix} 0 & 1 \\ 1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}$
- $BB^T = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$
- Solving $|B^T B - \lambda I| = 0$ we find $\lambda = \{1, 1, 0\}$

Pseudoinverse Exercise

Solution

- Corresponding eigenvectors $\begin{bmatrix}1\\0\\0\end{bmatrix}, \begin{bmatrix}0\\1\\0\end{bmatrix}, \begin{bmatrix}0\\0\\1\end{bmatrix}$

$$\hookrightarrow \Sigma = \begin{bmatrix}1 & 0 & 0\\0 & 1 & 0\end{bmatrix}, \quad V = \begin{bmatrix}1 & 0 & 0\\0 & 1 & 0\\0 & 0 & 1\end{bmatrix}, \quad U = \begin{bmatrix}1 & 0\\0 & 1\end{bmatrix}$$

- $B^\dagger = V\Sigma^\dagger U^T = \begin{bmatrix}1 & 0 & 0\\0 & 1 & 0\\0 & 0 & 1\end{bmatrix} \begin{bmatrix}1 & 0\\0 & 1\\0 & 0\end{bmatrix} \begin{bmatrix}0 & 1\\1 & 0\end{bmatrix} = \begin{bmatrix}0 & 1\\1 & 0\\0 & 0\end{bmatrix}$

- $C^TC = \begin{bmatrix}1 & 0\\1 & 0\end{bmatrix} \begin{bmatrix}1 & 1\\0 & 0\end{bmatrix} = \begin{bmatrix}1 & 1\\1 & 1\end{bmatrix}$

- $CC^T = \begin{bmatrix}1 & 1\\0 & 0\end{bmatrix} \begin{bmatrix}1 & 0\\1 & 0\end{bmatrix} = \begin{bmatrix}2 & 0\\0 & 0\end{bmatrix}$

Pseudoinverse Exercise

Solution

- Solving $|C^TC - \lambda I| = 0$ we find $\lambda = \{2, 0\}$, corresponding eigenvectors $\begin{bmatrix}1\\1\end{bmatrix}, \begin{bmatrix}-1\\1\end{bmatrix}$
- Solving $|CC^T - \lambda I| = 0$ we find $\lambda = \{2, 0\}$, corresponding eigenvectors $\begin{bmatrix}1\\0\end{bmatrix}, \begin{bmatrix}0\\1\end{bmatrix}$

$\hookrightarrow \Sigma = \begin{bmatrix}\sqrt{2} & 0\\0 & 0\end{bmatrix}, \quad U = \begin{bmatrix}1 & 0\\0 & 1\end{bmatrix}, \quad \begin{bmatrix}\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}}\\\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}\end{bmatrix}$

- $C^\dagger = V\Sigma^\dagger U^T = \begin{bmatrix}\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}}\\\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}\end{bmatrix}\begin{bmatrix}\frac{1}{\sqrt{2}} & 0\\0 & 0\end{bmatrix}\begin{bmatrix}1 & 0\\0 & 1\end{bmatrix} = \begin{bmatrix}\frac{1}{2} & 0\\\frac{1}{2} & 0\end{bmatrix}$

THANK YOU!

Slides available at:

`www.shpresimsadiku.com`

Check related information on Twitter at:

`@shpresimsadiku`