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Math Refresher for DS

Lecture 4

Last Time

- Matrices as linear transforms
- More on matrices
  - Rank
  - Determinant
  - Row / Column space
- Solving SLE

Today

- Matrix decompositions
- Eigenvalues & eigenvectors

Matrix Decomposition

- Factorization

$$21 = 3 \times 7$$

Matrix Decomposition

- Factorization

$$21 = 3 \times 7$$

- Matrix factorization: represent a matrix as a product of matrices with specific properties.

LU-Decomposition

LU Decomposition

- $A - n{\times}n$ matrix.
- Represent A as a product of two matrices:

$$A = LU, \text{ where}$$

$$L = \begin{pmatrix} l_{11} & 0 & \cdots & 0 \\ l_{21} & l_{22} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ l_{n1} & l_{n2} & \cdots & l_{nn} \end{pmatrix}, \qquad U = \begin{pmatrix} u_{11} & u_{12} & \cdots & u_{1n} \\ 0 & u_{22} & \cdots & u_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & u_{nn} \end{pmatrix}$$

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Reminder: Gaussian Elimination

$$A = \begin{pmatrix} -3 & 2 & -1 \\ 6 & -6 & 7 \\ 3 & -4 & 4 \end{pmatrix}$$

Elementary row operations:

$$\begin{pmatrix} -3 & 2 & -1 \\ 6 & -6 & 7 \\ 3 & -4 & 4 \end{pmatrix} \overset{(2)+2\cdot(1)}{\sim} \begin{pmatrix} -3 & 2 & -1 \\ 0 & -2 & 5 \\ 3 & -4 & 4 \end{pmatrix} \overset{(3)+1\cdot(1)}{\sim} \begin{pmatrix} -3 & 2 & -1 \\ 0 & -2 & 5 \\ 0 & -2 & 3 \end{pmatrix} \overset{(3)\ -1\cdot(2)}{\sim} \begin{pmatrix} 3 & 2 & -1 \\ 0 & -2 & 5 \\ 0 & 0 & -2 \end{pmatrix} = U -$$

an upper triangular matrix.

Key idea: elementary row operations can be represented as matrix operations!

Elementary Matrices

- Elementary row operations can be represented as matrix operations.

- We'll use **elementary matrices** like

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 2 & 0 & 1 \end{pmatrix}$$

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- Let's take a close look at our Gaussian elimination example.

Gaussian Elimination as Matrix Mult.

$$(2)' = (2) + 2 \cdot (1)$$

$$A = \begin{pmatrix} -3 & 2 & -1 \\ 6 & -6 & 7 \\ 3 & -4 & 4 \end{pmatrix} \sim \begin{pmatrix} -3 & 2 & -1 \\ 6 & -2 & 5 \\ 3 & -4 & 4 \end{pmatrix}$$

$$M_1 = \qquad\qquad , \quad \begin{pmatrix} -3 & 2 & -1 \\ 6 & -2 & 5 \\ 3 & -4 & 4 \end{pmatrix} = M_1 A$$

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$$M_2 = \qquad\qquad , \qquad \begin{pmatrix} -3 & 2 & -1 \\ 0 & -2 & 5 \\ 0 & -2 & 3 \end{pmatrix} = M_2 M_1 A$$

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$$M_3 M_2 M_1 A = U \Leftrightarrow \boldsymbol{A} = (M_3 M_2 M_1)^{-1} U$$

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$$M_3 M_2 M_1 A = U \Leftrightarrow \boldsymbol{A} = (M_3 M_2 M_1)^{-1} U = (M_1^{-1} M_2^{-1} M_3^{-1}) \boldsymbol{U}$$

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$$M_1 = \begin{pmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad M_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}, \quad M_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -1 & 1 \end{pmatrix}$$

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LU Decomposition: Application

- Solving SLE with different $\boldsymbol{b}$s:

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- Solving SLE with different bs:

$$Ax = b \Leftrightarrow (LU)x = b$$

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(1) $Ly = b \;\Leftrightarrow \qquad\qquad \rightarrow\; y^*$

(2) $Ux = y^* \Leftrightarrow \qquad\qquad \rightarrow x^*$ – solution to the original system.

LU Decomposition: Application

- Solving SLE with different bs:

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$$(1)\ Ly = b \ \Leftrightarrow \ \begin{array}{c} l_{11}\mathbf{y_1} = b_1 \\ l_{21}\mathbf{y_1} + l_{22}\mathbf{y_2} = b_2 \\ \vdots \\ l_{n1}y_1 + l_{n2}y_2 + \cdots + l_{nn}y_n = b_n \end{array} \ \rightarrow \ y^*$$

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$$(2)\ Ux = y^* \Leftrightarrow \begin{gathered} u_{11}x_1 + u_{12}x_2 + \cdots + u_{1n}x_n = y_1^* \\ u_{22}x_2 + \cdots + u_{1n}x_n = y_2^* \\ \vdots \\ u_{nn}\boldsymbol{x_n} = y_n^* \end{gathered} \ \rightarrow x^* - \text{solution to the original system.}$$

Eigenvalues & Eigenvectors

Eigenvectors and Eigenvalues

- Matrix A = some linear transformation.
- A changes vectors in V:

$$Ax = x'$$

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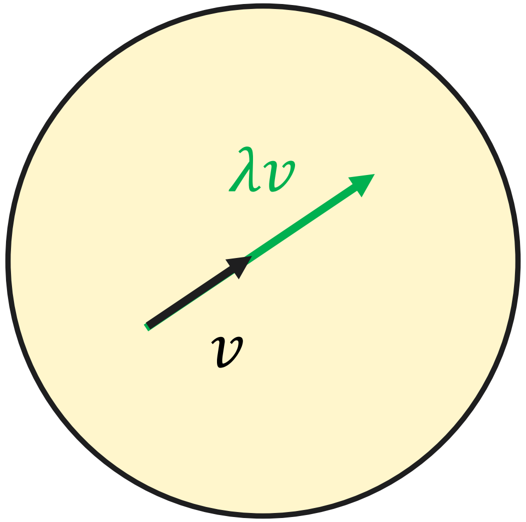

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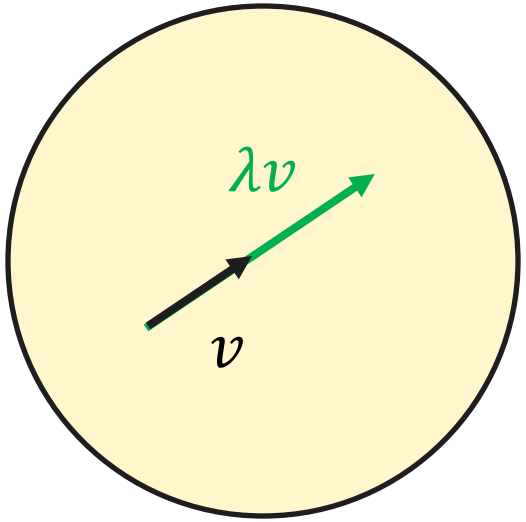


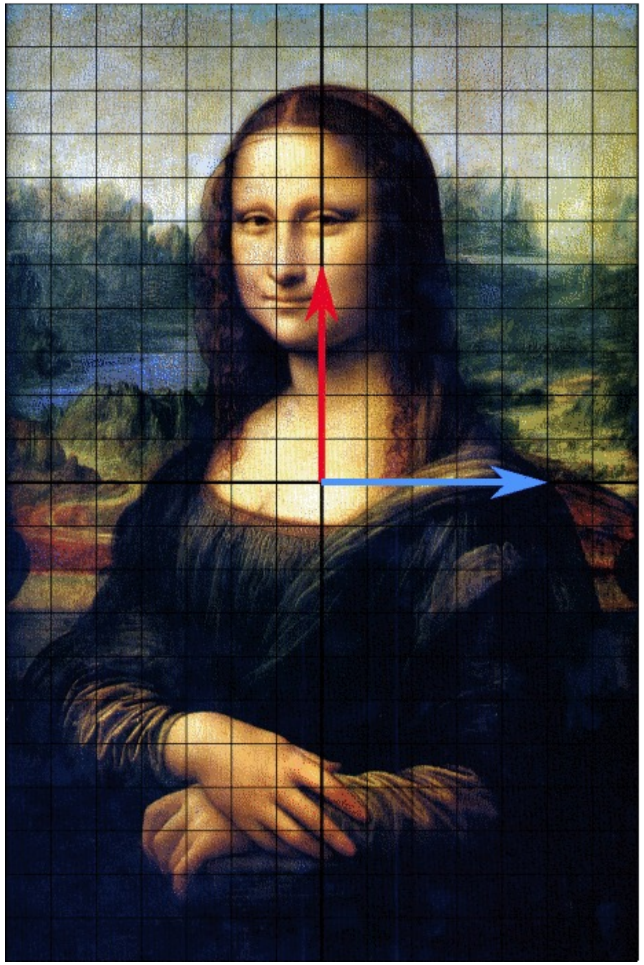
$$Av = \lambda v, \quad \lambda - \text{some number.}$$

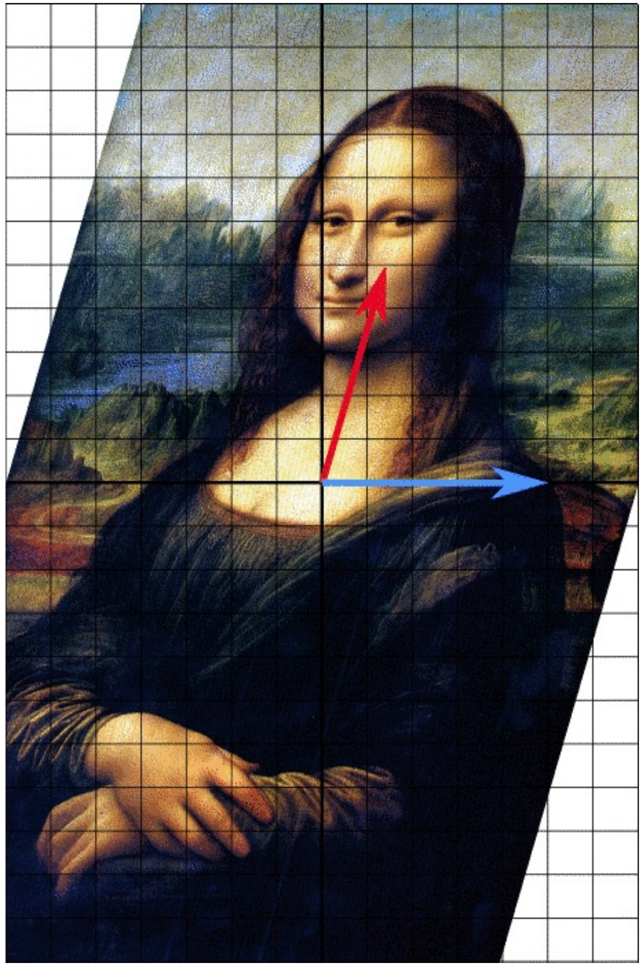
$\boldsymbol{\lambda}$ – eigenvalue, $\boldsymbol{v}$ – corresponding eigenvector

Eigenvectors and Eigenvalues

eigenvector = a vector that stays on its line after applying A and only gets stretched by λ.

Eigenvectors and Eigenvalues





Source: [Wikipedia]

Eigenvectors and Eigenvalues: Example 1

- Consider rotation in 3D.

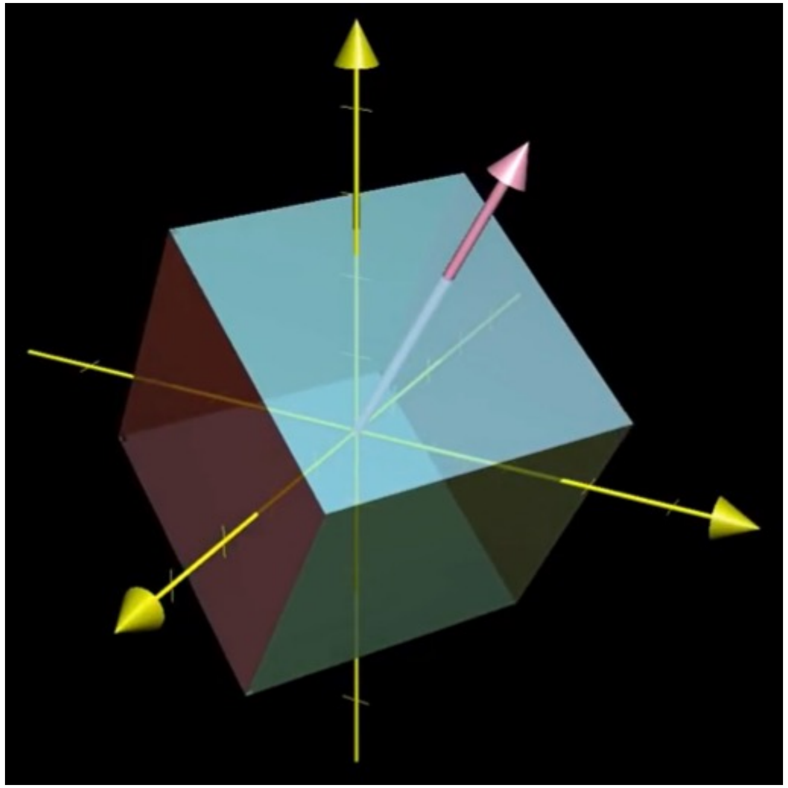
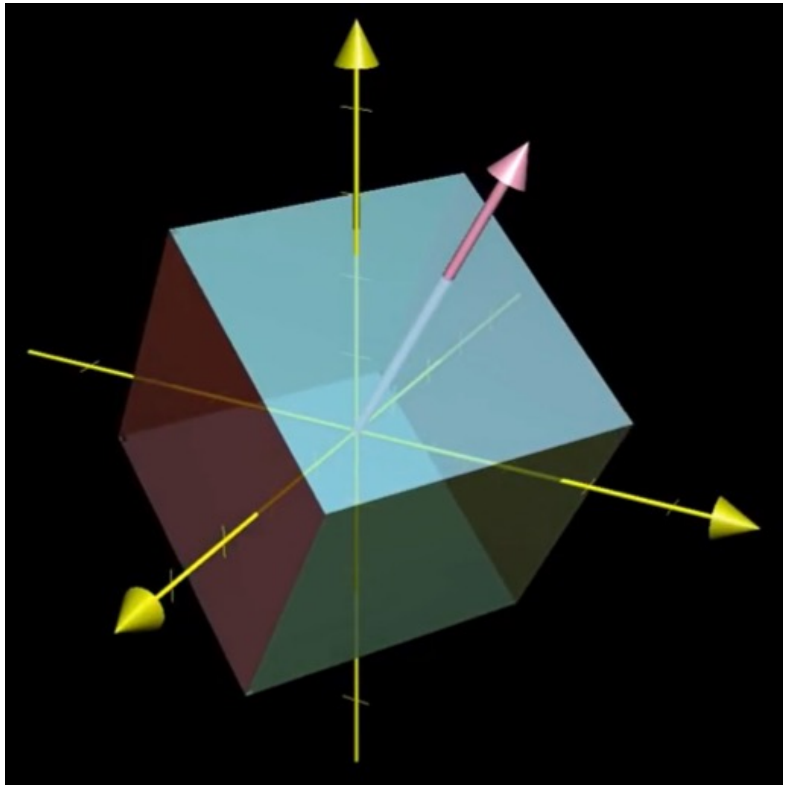


Image source:
http://andrewmacthoughts.blogspot.com/2019/05/visualizing-linear-algebra-eigenvectors.html

Eigenvectors and Eigenvalues: Example 1

- Consider rotation in 3D.

- Eigenvector =
  axis of the rotation.



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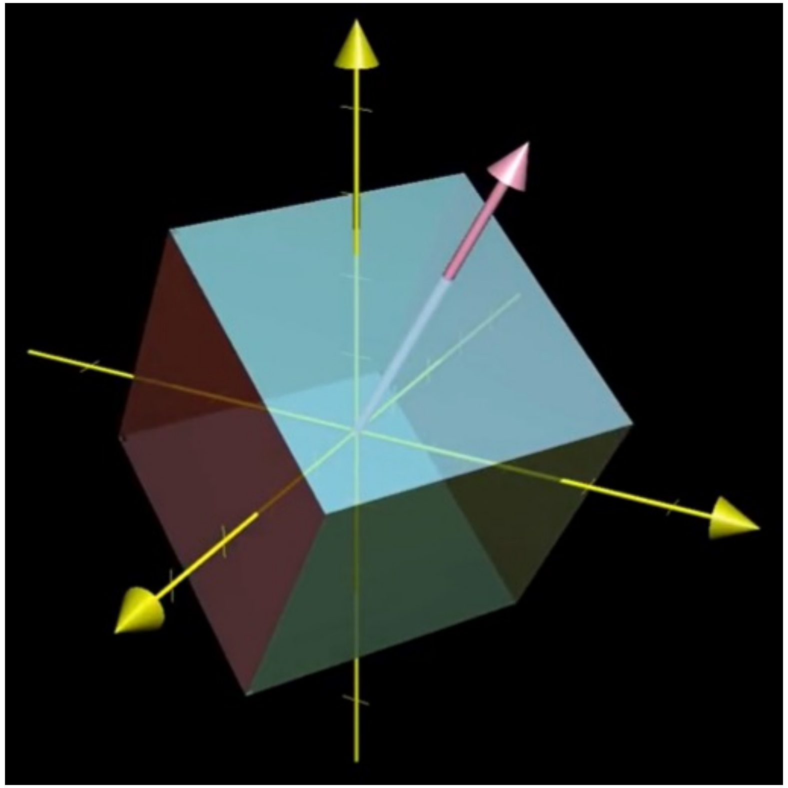
Eigenvectors and Eigenvalues: Example 1

- Consider rotation in 3D.
- Eigenvector = axis of the rotation.
- Corresponding eigenvalue is 1 (rotation doesn't change lengths)



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Eigenvectors and Eigenvalues: Example 2

- Consider a transformation $A = \begin{bmatrix} 3 & 1 \\ 0 & 2 \end{bmatrix}$.

Eigenvectors and Eigenvalues: Example 2

- Consider a transformation $\boldsymbol{A} = \begin{bmatrix} 3 & 1 \\ 0 & 2 \end{bmatrix}$.
- Basis vector $\boldsymbol{e_1} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ is an eigenvector with $\boldsymbol{\lambda_1} = 3$ *(see first column of* $\boldsymbol{A}$*).*

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Eigenvectors and Eigenvalues: Example 2

- Consider a transformation $A = \begin{bmatrix} 3 & 1 \\ 0 & 2 \end{bmatrix}$.

- Basis vector $\boldsymbol{e}_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ is an eigenvector with $\lambda_1 = 3$ *(see first column of A).*

- Vector $\boldsymbol{v} = \begin{bmatrix} -1 \\ 1 \end{bmatrix}$ is also an eigenvector! Indeed:

$$A\boldsymbol{v} = \begin{bmatrix} 3 & 1 \\ 0 & 2 \end{bmatrix} \begin{bmatrix} -1 \\ 1 \end{bmatrix} = \begin{bmatrix} -2 \\ 2 \end{bmatrix}, \qquad \lambda_2 = 2.$$

There Are Many Eigenvectors

- Let v be an eigenvector of A with the corresponding eigenvalue λ.

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- Note that $\forall\alpha \neq 0,\ \alpha \in R$ vector (αv) is also an eigenvector of A. Indeed,

$$A(\alpha v) = \alpha(Av) = \alpha\lambda v = \lambda(\alpha v)$$

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There Are Many Eigenvectors

- If v is an eigenvector, αv as well.

- Example:

$$A = \begin{bmatrix} 3 & 1 \\ 0 & 2 \end{bmatrix},\ e_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \text{ – eigenvector with } \lambda = 3.$$

There Are Many Eigenvectors

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- Example:

$$A = \begin{bmatrix} 3 & 1 \\ 0 & 2 \end{bmatrix},\ e_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \text{ – eigenvector with } \lambda = 3.$$

$$e'_1 = \begin{bmatrix} 10 \\ 0 \end{bmatrix} \text{ as well! Indeed: } \begin{bmatrix} 3 & 1 \\ 0 & 2 \end{bmatrix} \begin{bmatrix} 10 \\ 0 \end{bmatrix} = \begin{bmatrix} 30 \\ 0 \end{bmatrix} = 3 \begin{bmatrix} 10 \\ 0 \end{bmatrix}$$

Finding Eigenvalues & Eigenvectors

Finding Eigenvalues

- If v is an eigenvector with the corresponding eigenvalue λ, then

$$Av = \lambda v$$

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$$(A - \lambda E)v = 0$$

Since $v \neq \mathbf{0}$, this is only possible if and only if

$$\det(A - \lambda E) = 0$$

Finding Eigenvalues

- $v \neq 0$ is an eigenvector with the corresponding eigenvalue $\lambda \Leftrightarrow$

$$\det(A - \lambda E) = 0 \text{ –}$$

characteristic polynomial of A

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- Eigenvalues = roots of the characteristic polynomial:

$$\det(A - \lambda E) = a_n\lambda^n + a_{n-1}\lambda^{n-1} + \cdots + a_1\lambda + a_0 = 0 \Leftrightarrow$$

Polynomial of degree n = n (possibly repeating) roots:

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Polynomial of degree $\boldsymbol{n}$ = $\boldsymbol{n}$ (possibly repeating) roots:

$$(\lambda - \boldsymbol{\lambda_1})^{n_1} \cdot (\lambda - \boldsymbol{\lambda_2})^{n_2} \cdot \ldots \cdot (\lambda - \boldsymbol{\lambda_k})^{n_k} = 0, \qquad n_1 + \cdots + n_k = n$$

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$\{\boldsymbol{\lambda_1}, \ldots, \boldsymbol{\lambda_k}\}$ – spectrum of A.

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Finding Eigenvalues: Example 1

$$A = \begin{bmatrix} 3 & 1 \\ 0 & 2 \end{bmatrix}$$

Characteristic polynomial:

$$\det(A - \lambda E) = \begin{vmatrix} 3-\lambda & 1 \\ 0 & 2-\lambda \end{vmatrix} = (3-\lambda)(2-\lambda) = 0$$

$$\lambda_1 = 3, \qquad \lambda_2 = 2$$

Finding Eigenvectors: Example 1

$$A = \begin{bmatrix} 3 & 1 \\ 0 & 2 \end{bmatrix}, \qquad \lambda_1 = 3, \qquad \lambda_2 = 2$$

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$$\begin{bmatrix} 3-3 & 1 \\ 0 & 2-3 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 0 & -1 \end{bmatrix} \sim \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$$

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$$E_{\lambda_1} = \{v \in V \mid Av = \lambda_1 v\} = span\{v_1\}$$

Finding Eigenvectors: Example 1

$$A = \begin{bmatrix} 3 & 1 \\ 0 & 2 \end{bmatrix}, \qquad \lambda_1 = 3, \qquad \lambda_2 = 2$$

$$(A - \lambda_2 E)v_2 = 0$$

$$\begin{bmatrix} 3-2 & 1 \\ 0 & 2-2 \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ 0 & 0 \end{bmatrix}$$

Finding Eigenvectors: Example 1

$$A = \begin{bmatrix} 3 & 1 \\ 0 & 2 \end{bmatrix}, \qquad \lambda_1 = 3, \qquad \lambda_2 = 2$$

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$$\begin{bmatrix} 3-2 & 1 \\ 0 & 2-2 \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ 0 & 0 \end{bmatrix} \to v_2 = \begin{bmatrix} \beta \\ -\beta \end{bmatrix}, \text{ e.g. } v_2 = \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

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$$A = \begin{bmatrix} 3 & 1 \\ 0 & 2 \end{bmatrix}$$

$$\lambda_1 = 3, \qquad v_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \qquad \dim E_{\lambda_1} = 1$$

$$\lambda_2 = 2, \qquad v_2 = \begin{bmatrix} 1 \\ -1 \end{bmatrix}, \qquad \dim E_{\lambda_2} = 1$$

Finding Eigenvalues: Example 2

$$A = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

Characteristic polynomial:

$$\det(A - \lambda E) = \begin{vmatrix} 1 - \lambda & 0 \\ 0 & 1 - \lambda \end{vmatrix} = (1 - \lambda)^2 = 0$$

$$\lambda_{1,2} = \lambda = 1$$

Finding Eigenvalues: Example 2

$$A = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \qquad \lambda = 1$$

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$$\begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} v_i = 0 \iff v_{1,2} - \text{any vectors from } \mathbb{R}^2$$

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$$\text{e.g. } v_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, v_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

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e.g. $v_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, v_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$

$$E_\lambda = \{v \in V \mid Av = \lambda v\} = span\{v_1, v_2\} = \mathbb{R}^2$$

Finding Eigenvalues: Example 2

$$A = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$\lambda = 1, \qquad v_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, v_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \qquad \dim E_\lambda = 2$$

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Finding Eigenvalues: Example 3

$$A = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$$

Characteristic polynomial:

$$\det(A - \lambda E) = \begin{vmatrix} -\lambda & 1 \\ 0 & -\lambda \end{vmatrix} = \lambda^2 = 0$$

$$\lambda_{1,2} = \lambda = 0$$

Finding Eigenvalues: Example 3

$$A = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \qquad \lambda_{1,2} = \lambda = 0$$

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$$\begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} v_i = 0 \Leftrightarrow v = \begin{bmatrix} \alpha \\ 0 \end{bmatrix}, \text{e.g. } v = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

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Algebraic multiplicity = 2

$$E_\lambda = \{v \in V \mid Av = \lambda v\} = span\{v_1\}, \qquad \dim E_\lambda = 1$$

Geometric multiplicity = 1

λ – degenerate eigenvalue

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Useful Properties

- $A - n \times n$ matrix, $\lambda_1, \dots, \lambda_k$ – eigenvalues.
  - $\det A = \lambda_1 \cdot \ldots \cdot \lambda_k$

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  - $\mathbf{det}\,\boldsymbol{A} = \boldsymbol{\lambda_1} \cdot \ldots \cdot \boldsymbol{\lambda_k}$
  - $\mathbf{tr}\,\boldsymbol{A} = \boldsymbol{a_{11}} + \boldsymbol{a_{22}} + \cdots + \boldsymbol{a_{nn}} = \boldsymbol{\lambda_1} + \cdots + \boldsymbol{\lambda_k}$

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Useful Properties

- $A - n{\times}n$ matrix, $\lambda_1, \dots, \lambda_k$ – eigenvalues.

(1). $\boldsymbol{A}$ is invertible $\Leftrightarrow \boldsymbol{\lambda_i \neq 0, i = 1, \dots k}$:

Indeed, A is invertible $\Leftrightarrow 0 \neq \det A = \lambda_1 \cdot \dots \cdot \lambda_k$

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Indeed, A is invertible $\Leftrightarrow \mathbf{0} \neq \det A = \lambda_1 \cdot \dots \cdot \lambda_k$

(2). $\boldsymbol{A^{-1}}$ has eigenvalues $\boldsymbol{\frac{1}{\lambda_1}, \dots, \frac{1}{\lambda_k}}$.

(Eigenvectors of $\boldsymbol{A}$ and $\boldsymbol{A^{-1}}$ are the same:

$$Av_i = \lambda_i v_i \Leftrightarrow v_i = \lambda_i A^{-1} v_i \Leftrightarrow \frac{1}{\lambda_i} v_i = A^{-1} v_i$$

Eigen-decomposition

Eigenbasis

- $A - n{\times}n$ matrix.
- Suppose that A has n linearly independent eigenvectors $v_1, \dots, v_n$.

$$\{\boldsymbol{v_1}, \dots, \boldsymbol{v_n}\} \text{ – eigenbasis.}$$

Eigendecomposition

- $A - n{\times}n$ matrix, $v_1, \dots, v_n$ - linearly independent eigenvectors, $\lambda_1, \dots, \lambda_n -$ corresponding eigenvalues.
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Eigendecomposition

- $A - n\times n$ matrix, $v_1, \dots, v_n$ - linearly independent eigenvectors, $\lambda_1, \dots, \lambda_n -$ corresponding eigenvalues.

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$$V = [v_1 \mid v_2 \mid \dots \mid v_n] - \text{change-of-basis matrix}$$

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$$A = V[A]_V V^{-1}$$

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$$= \begin{bmatrix} \lambda_1 & 0 & 0 & 0 \\ 0 & \lambda_2 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \lambda_n \end{bmatrix} = \Lambda \text{ – a diagonal matrix.}$$

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$V = [v_1 \mid v_2 \mid \dots \mid v_n]$ – change-of-basis matrix

$$A = V[A]_V V^{-1}$$

$[A]_V = \Lambda$ – a diagonal matrix with $d_{ii} = \lambda_i$

$\boldsymbol{A = V\Lambda V^{-1}}$ – eigendecomposition of $\boldsymbol{A}$.

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Matrix Diagonalization

Diagonalizable Matrix

- $A - n{\times}n$ matrix
- $v_1, \dots, v_n$ - linearly independent eigenvectors
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Eigendecomposition of $\boldsymbol{A}$: $\boldsymbol{A} = \boldsymbol{V\Lambda V^{-1}}$ –

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Eigendecomposition of $\boldsymbol{A}$: $\boldsymbol{A} = \boldsymbol{V\Lambda V^{-1}}$ –

$$\Leftrightarrow$$

Diagonalization of $\boldsymbol{A}$: $\boldsymbol{\Lambda} = \boldsymbol{V^{-1}AV}$

Matrix Diagonalization: Example

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$v_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, v_2 = \begin{bmatrix} -1 \\ 1 \end{bmatrix}$ – corresponding eigenvectors

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$$\Lambda = \begin{bmatrix} 1 & -1 \\ 0 & 1 \end{bmatrix}^{-1} \begin{bmatrix} 3 & 1 \\ 0 & 2 \end{bmatrix} \begin{bmatrix} 1 & -1 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 3 & 1 \\ 0 & 2 \end{bmatrix} \begin{bmatrix} 1 & -1 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 3 & 0 \\ 0 & 2 \end{bmatrix}$$

Diagonalizable Matrix

- But now all matrices have n linearly independent eigenvectors.

- Example (see beginning of the lecture):

$$A = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \qquad \lambda_{1,2} = \lambda = 0, \qquad v = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

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So, when is a matrix diagonalizable?

The Spectral Theorem

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  2. A has n linearly independent eigenvectors $v_1, \dots, v_n$;
  3. $v_1, \dots, v_n$ are orthogonal *(we can chose orthonormal)*.

Orthogonal Matrices

- $A - n \times n$ matrix
- A is orthogonal if its columns are mutually orthonormal:

$$A^T A = A A^T = E$$

Orthogonal Matrices

- Suppose that A is orthogonal.
- Orthogonal vectors are linearly independent → A is a full rank matrix. So, A has an inverse!

$$A \text{ is orthogonal} \Leftrightarrow$$
$$A^T A = AA^T = E \Leftrightarrow$$
$$A^{-1} = A^T.$$

The Spectral Theorem

In other words, if $\boldsymbol{A}$ is a real symmetric matrix,
$\boldsymbol{A}$ is orthogonally diagonalizable:

$$\boldsymbol{\Lambda} = \boldsymbol{V}^{-1}\boldsymbol{A}\boldsymbol{V} = \boldsymbol{V}^{T}\boldsymbol{A}\boldsymbol{V}$$

where $\boldsymbol{\Lambda}$ is a diagonal matrix and $\boldsymbol{V}$ is an orthogonal matrix.

Power of a Matrix

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- Let A be an $n \times n$ matrix. Imagine that you need to compute A^n. How to do it efficiently?

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- Let A be an $n{\times}n$ matrix. Imagine that you need to compute A^n. How to do it efficiently?

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$$A^n = V\Lambda^n V^{-1}$$

$$\Lambda^n = \begin{bmatrix} \lambda_1^n & 0 & \cdots & 0 \\ 0 & \lambda_2^n & \cdots & 0 \\ \vdots & \vdots & \cdots & \vdots \\ 0 & 0 & \cdots & \lambda_m^n \end{bmatrix}$$

Principle Component Analysis

PCA

- Principle Component Analysis (PCA) - a powerful statistical tool for analyzing data based on eigendecomposition.

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- Suppose you have a dataset with n observations and m features:

$$\mathrm{x}^{\mathrm{j}} = \begin{bmatrix} x_{1j} \\ x_{2j} \\ \vdots \\ x_{mj} \end{bmatrix} - \text{observations for example } j, \ \boldsymbol{X} = \left[\mathbf{x}^{1} \mid \ldots \mid \mathbf{x}^{n}\right] - m \times n \text{ data matrix.}$$

PCA

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- Suppose you have a dataset with n observations and m features:

$$\mathrm{x}^{\mathrm{j}} = \begin{bmatrix} x_{1j} \\ x_{2j} \\ \vdots \\ x_{mj} \end{bmatrix}$$ – observations for example j, $\boldsymbol{X} = [\mathbf{x}^{\mathbf{1}} \mid \dots \mid \mathbf{x}^{\boldsymbol{n}}]$ – $m \times n$ data matrix.

- You might be wondering
    - is there a way to visualize the data?
    - which features are the most significant in describing the full dataset?

PCA

- Principle Component Analysis (PCA) - a powerful statistical tool for analyzing data based on eigendecomposition.

- Suppose you have a dataset with $\boldsymbol{n}$ observations and $\boldsymbol{m}$ features:

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PCA

- Key idea: project your $\boldsymbol{m} \times \boldsymbol{n}$ data onto a $\boldsymbol{p}$-dimensional subspace ($\boldsymbol{p} < \boldsymbol{m}$) in such a way that we preserve as much variance in our data as possible.

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- Suppose that this subspace has an orthonormal basis $B = [b^1 \mid \ldots \mid b^p]$. Then

$$X_{proj} = BX$$

girafe ai

PCA

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- Suppose that this subspace has an orthonormal basis $B = [b^1 \mid \dots \mid b^p]$. Then

$$X_{proj} = B^T X$$

How to find B?

Turns out we should project on the $\boldsymbol{p}$ eigenvectors of the data covariance matrix that correspond to $\boldsymbol{p}$ largest eigenvalues!

PCA

- *(Probability Theory)* Covariance between two random variables = measure of the joint variability.
- We have a dataset X:

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Assuming that X is centered, otherwise we should center it first.

- *(Statistics)* Sample covariance matrix: $S = \frac{1}{n-1} X X^T$

$s_{ij},\ i \neq j$ – sample covariance between features i and j,

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PCA

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$$\frac{1}{n-1} X X^T = S = V \Lambda V^{-1} = V \Lambda V^T$$

$V = [v_1 \mid \ldots \mid v_m]$ – eigenvectors of S, Λ – diagonal matrix with λ_i.

PCA

- Let's order eigenvalues and eigenvectors so that $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_m$.

$$S = V\Lambda V^{-1} = V\Lambda V^T$$

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Total variance of the data $\mathrm{T} = tr(S) = s_{11} + \cdots + s_{nn}$

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Orthogonal eigenvectors $v_1, \ldots, v_n$ – **principal components** of the data

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Direction of v_i describes λ_i out of the total variance T.

To Sum Up

- Eigenvalues and eigenvectors

- Matrix factorization
  - LU
  - Eigendecomposition
  - Diagonalization