

## 23. Singular Value Decomposition (SVD) and eigen-decomposition

## Last time

- Least squares
- Optimization
- Solution by linear algebra
- Pseudo-inverse

## Goals for today

- Action of a matrix
- Eigenvector decomposition
- Singular Value Decomposition (SVD)

## Action of a matrix

- Consider arbitrary  $(m \times n)$  matrix  $A$

## Action of a matrix

- Consider arbitrary  $(m \times n)$  matrix  $A$
- Study its action on unit sphere  $\mathbb{S}_n$  in  $\mathbb{R}^n$
- $\mathbb{S}_n := \{\mathbf{x} \in \mathbb{R}^n : \|\mathbf{x}\|_2 = 1\}$

## Action of a matrix

- Consider arbitrary  $(m \times n)$  matrix  $A$
- Study its action on unit sphere  $\mathbb{S}_n$  in  $\mathbb{R}^n$
- $\mathbb{S}_n := \{\mathbf{x} \in \mathbb{R}^n : \|\mathbf{x}\|_2 = 1\}$
- Visualization suggests  $A(\mathbb{S}_n)$  is **ellipsoid** (hyper-ellipse)
- Stretched and rotated sphere

## Action of a matrix

- Consider arbitrary  $(m \times n)$  matrix  $A$
- Study its action on unit sphere  $\mathbb{S}_n$  in  $\mathbb{R}^n$
- $\mathbb{S}_n := \{\mathbf{x} \in \mathbb{R}^n : \|\mathbf{x}\|_2 = 1\}$
  
- Visualization suggests  $A(\mathbb{S}_n)$  is **ellipsoid** (hyper-ellipse)
- Stretched and rotated sphere
  
- Key quantities:
  - Lengths  $\sigma_i$  of semi-axes – amount of stretch
  - Directions  $\mathbf{u}_i$  of stretches

## Action of a matrix II

- Let's try to understand how this comes about:



## Action of a matrix II

- Let's try to understand how this comes about:
- Suppose  $\mathbf{x} \in \mathbb{S}_n$ ; define  $\mathbf{y} := A\mathbf{x}$  to be its image

## Action of a matrix II

- Let's try to understand how this comes about:
- Suppose  $\mathbf{x} \in \mathbb{S}_n$ ; define  $\mathbf{y} := A\mathbf{x}$  to be its image
- Suppose that  $A$  square + invertible for now

## Action of a matrix II

- Let's try to understand how this comes about:
- Suppose  $\mathbf{x} \in \mathbb{S}_n$ ; define  $\mathbf{y} := A\mathbf{x}$  to be its image
- Suppose that  $A$  square + invertible for now
- Then  $\|A^{-1}\mathbf{y}\|^2 = 1$

## Action of a matrix II

- Let's try to understand how this comes about:
- Suppose  $\mathbf{x} \in \mathbb{S}_n$ ; define  $\mathbf{y} := A\mathbf{x}$  to be its image
- Suppose that  $A$  square + invertible for now
- Then  $\|A^{-1}\mathbf{y}\|^2 = 1$
- Hence

$$\mathbf{y}^\top S \mathbf{y} = 1$$

where  $S := (A^{-1})^\top (A^{-1})$  is symmetric + positive definite

# Eigenvalues

- Recall: square  $m \times m$  matrix  $M$  has **eigenvector**  $\mathbf{v} \neq \mathbf{0}$  with **eigenvalue**  $\lambda \in \mathbb{C}$  if

$$M\mathbf{v} = \lambda\mathbf{v}$$

# Eigenvalues

- Recall: square  $m \times m$  matrix  $M$  has **eigenvector**  $\mathbf{v} \neq \mathbf{0}$  with **eigenvalue**  $\lambda \in \mathbb{C}$  if

$$M\mathbf{v} = \lambda\mathbf{v}$$

- Geometrical meaning: Direction  $\hat{\mathbf{v}}$  is **invariant** (unchanged) under  $A$
- *Stretched* (and possibly reflected) by factor  $\lambda$

## Spectral theorem

- **Spectrum** of matrix: set of eigenvalues

## Spectral theorem

- **Spectrum** of matrix: set of eigenvalues
- Eigenvalues satisfy  $\det(A - \lambda I) = 0$  – **characteristic polynomial**
- Fundamental thm of algebra  $\implies$  there are  $m$  eigenvalues
- For a real, **symmetric** matrix  $S$ , *exercise*:
  - eigenvalues  $\lambda_i$  are **real**
  - eigenvectors  $\mathbf{v}_i$  with *distinct*  $\lambda_i$  are **orthogonal**



## Spectral theorem

- **Spectrum** of matrix: set of eigenvalues
- Eigenvalues satisfy  $\det(A - \lambda I) = 0$  – **characteristic polynomial**
- Fundamental thm of algebra  $\implies$  there are  $m$  eigenvalues
- For a real, **symmetric** matrix  $S$ , *exercise*:
  - eigenvalues  $\lambda_i$  are **real**
  - eigenvectors  $\mathbf{v}_i$  with *distinct*  $\lambda_i$  are **orthogonal**
- “Hence” **spectral theorem**: real symmetric matrices have a basis of orthonormal eigenvectors

## Spectral theorem

- **Spectrum** of matrix: set of eigenvalues
- Eigenvalues satisfy  $\det(A - \lambda I) = 0$  – **characteristic polynomial**
- Fundamental thm of algebra  $\implies$  there are  $m$  eigenvalues
- For a real, **symmetric** matrix  $S$ , *exercise*:
  - eigenvalues  $\lambda_i$  are **real**
  - eigenvectors  $\mathbf{v}_i$  with *distinct*  $\lambda_i$  are **orthogonal**
- “Hence” **spectral theorem**: real symmetric matrices have a basis of orthonormal eigenvectors

# Eigen-decomposition

- Have  $SQ = Q\Lambda$ , where

$$Q := (\mathbf{v}_1 | \mathbf{v}_2 | \cdots | \mathbf{v}_n)$$

$$\Lambda := \begin{bmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_m \end{bmatrix}$$

# Eigen-decomposition

- Have  $SQ = Q\Lambda$ , where

$$Q := (\mathbf{v}_1 | \mathbf{v}_2 | \cdots | \mathbf{v}_n)$$

$$\Lambda := \begin{bmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_m \end{bmatrix}$$

- Hence  $S = Q\Lambda Q^\top$

## Action of a matrix III

■ So  $\mathbf{y}^\top \mathbf{Q} \mathbf{\Lambda} \mathbf{Q}^\top \mathbf{y} = 1$

## Action of a matrix III

- So  $\mathbf{y}^\top \mathbf{Q} \mathbf{\Lambda} \mathbf{Q}^\top \mathbf{y} = 1$

- Hence  $\mathbf{z}^\top \mathbf{\Lambda} \mathbf{z} = 1$

where  $\mathbf{z} := \mathbf{Q}^\top \mathbf{y}$

## Action of a matrix III

- So  $\mathbf{y}^\top \mathbf{Q} \mathbf{\Lambda} \mathbf{Q}^\top \mathbf{y} = 1$
- Hence  $\mathbf{z}^\top \mathbf{\Lambda} \mathbf{z} = 1$   
where  $\mathbf{z} := \mathbf{Q}^\top \mathbf{y}$
- So  $\lambda_1 z_1^2 + \dots + \lambda_n z_n^2 = 1$

## Action of a matrix III

- So  $\mathbf{y}^\top \mathbf{Q} \mathbf{\Lambda} \mathbf{Q}^\top \mathbf{y} = 1$
- Hence  $\mathbf{z}^\top \mathbf{\Lambda} \mathbf{z} = 1$   
 where  $\mathbf{z} := \mathbf{Q}^\top \mathbf{y}$
- So  $\lambda_1 z_1^2 + \dots + \lambda_n z_n^2 = 1$
- Can show  $(\mathbf{A}^\top \mathbf{A})^{-1}$  has eigenvalues  $\lambda_i > 0$  (exercise)



## Action of a matrix III

- So  $\mathbf{y}^\top \mathbf{Q} \mathbf{\Lambda} \mathbf{Q}^\top \mathbf{y} = 1$
- Hence  $\mathbf{z}^\top \mathbf{\Lambda} \mathbf{z} = 1$   
 where  $\mathbf{z} := \mathbf{Q}^\top \mathbf{y}$
- So  $\lambda_1 z_1^2 + \dots + \lambda_n z_n^2 = 1$
- Can show  $(\mathbf{A}^\top \mathbf{A})^{-1}$  has eigenvalues  $\lambda_i > 0$  (exercise)
- Hence  $\mathbf{z}$  lies on ellipse  
 with semi-axis lengths  $\sigma_i := \sqrt{\lambda_i}$
- $\mathbf{y}$  lies on rotated ellipse

## Singular values and singular vectors

- $\sigma_i$  are **singular values** of A [terrible name]

## Singular values and singular vectors

- $\sigma_i$  are **singular values** of  $A$  [terrible name]
- Directions  $\mathbf{u}_i$ , columns of  $Q$ , are **left singular vectors**
  - directions in which ellipse is stretched
- $\mathbf{v}_i$  such that  $A\mathbf{v}_i = \sigma_i\mathbf{u}_i$  are **right singular vectors**

## Singular-value decomposition (SVD)

- Any  $(m \times n)$  matrix  $A$  has an SVD:

$$A = U\Sigma V^T$$

- columns of  $U$  are  $\mathbf{u}_i$
- columns  $V$  are  $\mathbf{v}_i$
- $\Sigma$  is diagonal matrix with  $\sigma_i$  on diagonal

## Singular-value decomposition (SVD)

- Any  $(m \times n)$  matrix  $A$  has an SVD:

$$A = U\Sigma V^T$$

- columns of  $U$  are  $\mathbf{u}_i$
- columns  $V$  are  $\mathbf{v}_i$
- $\Sigma$  is diagonal matrix with  $\sigma_i$  on diagonal
- Geometrical interpretation:

## Calculating eigenvalues

- As usual, still don't know how to actually *calculate* anything!

## Calculating eigenvalues

- As usual, still don't know how to actually *calculate* anything!
- Need to calculate eigenvalues  $\lambda_i$  and eigenvectors  $\mathbf{v}_i$  of symmetric matrix  $S$

## Calculating eigenvalues

- As usual, still don't know how to actually *calculate* anything!
- Need to calculate eigenvalues  $\lambda_i$  and eigenvectors  $\mathbf{v}_i$  of symmetric matrix  $S$
- Note: there are direct methods for the singular values  $\sigma_i$  that avoid  $\mathbf{g} \mathbf{A}^\top \mathbf{A}$



## Power iteration method

- Simple method to get eigenvector with largest eigenvalue, **leading** eigenvector

## Power iteration method

- Simple method to get eigenvector with largest eigenvalue, **leading** eigenvector
- Start with any initial  $\mathbf{v} \neq \mathbf{0}$

## Power iteration method

- Simple method to get eigenvector with largest eigenvalue, **leading** eigenvector
- Start with any initial  $\mathbf{v} \neq \mathbf{0}$
- Apply  $A$  repeatedly to form  $A^n \mathbf{v}$
- In general will explode, so normalize
- Converges to leading eigenvector!

## Power iteration method

- Simple method to get eigenvector with largest eigenvalue, **leading** eigenvector
- Start with any initial  $\mathbf{v} \neq \mathbf{0}$
- Apply  $A$  repeatedly to form  $A^n \mathbf{v}$
- In general will explode, so normalize
- Converges to leading eigenvector!
- To see this expand  $\mathbf{v}$  in basis of eigenvectors

## Simultaneous power method

- Suppose start with several vectors  $\mathbf{v}_1, \dots, \mathbf{v}_k$
- If iterate each separately, all will converge to leading eigenvector

## Simultaneous power method

- Suppose start with several vectors  $\mathbf{v}_1, \dots, \mathbf{v}_k$
- If iterate each separately, all will converge to leading eigenvector
- Solution: Orthogonalize using Gram–Schmidt

## Simultaneous power method

- Suppose start with several vectors  $\mathbf{v}_1, \dots, \mathbf{v}_k$
- If iterate each separately, all will converge to leading eigenvector
- Solution: Orthogonalize using Gram–Schmidt
- Converge to leading  $k$  eigenvectors

## Simultaneous power method

- Suppose start with several vectors  $\mathbf{v}_1, \dots, \mathbf{v}_k$
- If iterate each separately, all will converge to leading eigenvector
- Solution: Orthogonalize using Gram–Schmidt
- Converge to leading  $k$  eigenvectors
- This is part of QR algorithm:
  - 1 Factorize  $QR = A$
  - 2 Set  $A \leftarrow RQ$
  - 3 Repeat



## Simultaneous power method

- Suppose start with several vectors  $\mathbf{v}_1, \dots, \mathbf{v}_k$
- If iterate each separately, all will converge to leading eigenvector
- Solution: Orthogonalize using Gram–Schmidt
- Converge to leading  $k$  eigenvectors
- This is part of QR algorithm:
  - 1 Factorize  $QR = A$
  - 2 Set  $A \leftarrow RQ$
  - 3 Repeat
- $A$  converges to diagonal matrix of eigenvalues!

## Rank of a matrix

- Number of non-zero singular values = column rank = rank

## Rank of a matrix

- Number of non-zero singular values = column rank = rank
- SVD gives **best approximation** to A by matrix of rank  $k$ :

$$A_k := \sum_{i=1}^k \sigma_i \mathbf{u}_i \mathbf{v}_i^T$$

## Rank of a matrix

- Number of non-zero singular values = column rank = rank
- SVD gives **best approximation** to  $A$  by matrix of rank  $k$ :

$$A_k := \sum_{i=1}^k \sigma_i \mathbf{u}_i \mathbf{v}_i^T$$

- Use to find low-rank approximation of collection of data – PCA (Principal Component Analysis in statistics)
- E.g. image compression

# Summary

- SVD gives matrix as rotation + stretch + rotation
- Closely related to eigendecomposition of  $A^T A$

# Summary

- SVD gives matrix as rotation + stretch + rotation
- Closely related to eigendecomposition of  $A^T A$
- Applications to data summarization compression