Mathematics Methods for Computer Science

Statistical Motivation

**Properties** 

Spectral Theorem

Other

**ODE Theory** 

Spectral Embedding

# Mathematics Methods for Computer Science

Instructor: Xubo Yang

SJTU-SE DALAB



Mathematics Methods for Computer Science

Statistical Motivation

Properties

Spectral Theorem

Other

**ODE Theor** 

Spectral Embedding

### Lecture

# Eigenproblems I

# Setup

Statistical Motivation

Propertie:

Spectral Theore

Other

ODE Theor

Spectral Embedding

# **Given:** Collection of data points $\vec{x}_i$

- Age
- Weight
- Blood pressure
- Heart rate

# Setup

Statistical Motivation

Propertie:

Spectral Theore

Other

**ODE Theor** 

Constant Foots at

**Given:** Collection of data points  $\vec{x}_i$ 

- Age
- Weight
- Blood pressure
- Heart rate

**Find:** Correlations between different dimensions

# Simplest Model

#### Statistical Motivation

**Properties** 

Spectral Theore

Other

ODE Theor

Spectral Embedding

# **One-dimensional subspace**

$$ec{x}_i pprox c_i ec{v}, ec{v}$$
 unknown

# Simplest Model

#### Statistical Motivation

Propertie:

Spectral Theorer

Othei

ODE Theor

Spectral Embedding

# **One-dimensional subspace**

 $\vec{x}_i \approx c_i \vec{v}, \vec{v}$  unknown

# **Equivalently:**

$$\vec{x}_i \approx c_i \hat{v}$$

$$\hat{v}$$
 unknown with  $||\hat{v}||_2 = 1$ 

### Variational Idea

Statistical Motivation

**Properties** 

Spectral Theorer

Other

ODE Theor

$$minimize_{\hat{v}}\sum_{i}||\vec{x}_{i}-proj_{\hat{v}}\vec{x}_{i}||_{2}^{2}$$
 such that  $||\hat{v}||_{2}=1$ 

### Variational Idea

Statistical Motivation

Properties

Spectral Theoren

Other

ODE Theor

Spectral Embedding

$$minimize_{\hat{v}} \sum_i ||\vec{x}_i - proj_{\hat{v}}\vec{x}_i||_2^2$$
 such that  $||\hat{v}||_2 = 1$ 

What does the constraint do?

### Variational Idea

Statistical Motivation

Propertie:

Spectral Theorer

Othei

ODE Theor

Spectral Embedding

$$minimize_{\hat{v}} \sum_i ||\vec{x}_i - proj_{\hat{v}}\vec{x}_i||_2^2$$
 such that  $||\hat{v}||_2 = 1$ 

## What does the constraint do?

- ullet Does not affect optimal  $\hat{v}$
- Removes scaling ambiguity

Mathematics Methods for Computer Science

# Geometric Interpretation

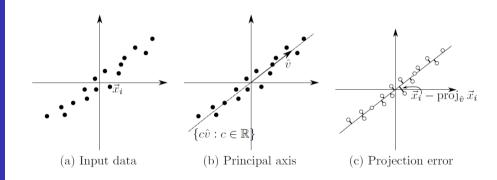
Statistical Motivation

Properties

Spectral Theorem

Othe

ODE Theor



### Review from Last Lecture

Statistical Motivation

**Properties** 

Spectral Theoren

Other

ODE Theor

Spectral Embedding

$$min_{c_i}||\vec{x}_i - c_i\hat{v}||_2$$

What is  $c_i$  ?

### Review from Last Lecture

Statistical Motivation

Properties

Spectral Theorer

Other

ODE Theor

Spectral Embedding

$$min_{c_i}||\vec{x}_i - c_i\hat{v}||_2$$

# What is $c_i$ ?

$$c_i = \vec{x}_i \cdot \hat{v}$$

# **Equivalent Optimization**

Statistical Motivation

Propertie:

Spectral Theorer

Other

**ODE Theor** 

maximize 
$$||X^T\hat{v}||_2^2$$
 such that  $||\hat{v}||_2^2=1$ 

### **End Goal**

Statistical Motivation

Properties

Spectral Theore

Other

ODE Theor

Spectral Embedding

Eigenvector of  $XX^T$  with largest eigenvalue.

Statistical Motivation

Propertie:

Spectral Theorer

Other

ODE Theor

Spectral Embedding

Eigenvector of  $XX^T$  with largest eigenvalue.

"First principal component"

More after SVD!

### Definitions

Statistical Motivation

**Properties** 

Spectral Theorer

Othe

ODE Theory

Spectral Embedding

### Eigenvalue and eigenvector

An eigenvector  $\vec{x} \neq \vec{0}$  of  $A \in \mathbb{R}^{n \times n}$  satisfies

 $A\vec{x}=\lambda\vec{x}$  for some  $\lambda\in\mathbb{R}$ ;  $\lambda$  is an eigenvalue.

Complex eigenvalues and eigenvectors instead have

 $\lambda \in \mathbb{C}$  and  $\vec{x} \in \mathbb{C}^n$ .

### **Definitions**

Statistical Motivation

**Properties** 

Spectral Theorer

Other

ODE Theor

Spectral Embedding

### Eigenvalue and eigenvector

An eigenvector  $\vec{x} \neq \vec{0}$  of  $A \in \mathbb{R}^{n \times n}$  satisfies  $A\vec{x} = \lambda \vec{x}$  for some  $\lambda \in \mathbb{R}$ ;  $\lambda$  is an eigenvalue. Complex eigenvalues and eigenvectors instead have  $\lambda \in \mathbb{C}$  and  $\vec{x} \in \mathbb{C}^n$ .

### Scale doesn't matter!

$$\rightarrow$$
 can constrain  $||\vec{x}||_2 \equiv 1$ 

# Eigenproblems in the Wild

Statistical Motivation

**Properties** 

Spectral Theore

Othe

ODE Theor

Spectral Embedding

• Optimize  $||A\vec{x}||_2$  such that  $||\vec{x}||_2 = 1$  (important!)

## Eigenproblems in the Wild

Statistical Motivation

**Properties** 

Spectral Theore

Othe

ODE Theor

- Optimize  $||A\vec{x}||_2$  such that  $||\vec{x}||_2 = 1$  (important!)
- $\bullet$  ODE/PDE problems: Closed solutions and approximations for  $\vec{y}'=B\vec{y}$

# Eigenproblems in the Wild

Statistical Motivation

**Properties** 

Spectral Theore

Othe

ODE Theor

- Optimize  $||A\vec{x}||_2$  such that  $||\vec{x}||_2 = 1$  (important!)
- $\bullet$  ODE/PDE problems: Closed solutions and approximations for  $\vec{y}'=B\vec{y}$
- Critical points of Rayleigh quotient:

$$\frac{\vec{x}^T A \bar{x}}{||\vec{x}||_2^2}$$

# Two Basic Properties

Proved in textbook

Statistical Motivation

**Properties** 

Spectral Theoren

Other

ODE Theor

Spectral Embedding

#### Lemma

Every matrix  $A \in \mathbb{R}^{n \times n}$  has at least one (complex) eigenvector.

## Two Basic Properties

Proved in textbook

Statistical Motivation

**Properties** 

Spectral Theorer

Other

ODE Theory

Spectral Embeddin

#### Lemma

Every matrix  $A \in \mathbb{R}^{n \times n}$  has at least one (complex) eigenvector.

#### Lemma

Eigenvectors corresponding to distinct eigenvalues must be linearly independent.

## Two Basic Properties

Proved in textbook

Statistical Motivation

**Properties** 

Spectral Theorer

Other

ODE Theor

Spectral Embeddin

#### Lemma

Every matrix  $A \in \mathbb{R}^{n \times n}$  has at least one (complex) eigenvector.

#### Lemma

Eigenvectors corresponding to distinct eigenvalues must be linearly independent.

 $\rightarrow$  at most n eigenvalues

# Diagonalizability

Statistical Motivation

**Properties** 

Spectral Theorer

Othe

ODE Theor

. . . . . .

#### Nondefective

 $A \in \mathbb{R}^{n \times n}$  is nondefective or diagonalizable if its eigenvectors span  $\mathbb{R}^n$ .

# Diagonalizability

Statistical Motivation

**Properties** 

Spectral Theore

Othe

ODE Theory

Spectral Embeddin

#### Nondefective

 $A \in \mathbb{R}^{n \times n}$  is nondefective or diagonalizable if its eigenvectors span  $\mathbb{R}^n$ .

$$D = X^{-1}AX$$

A is diagonalized by a similarity transformation  $A \to X^{-1}AX$ 

### Definitions

Statistical Motivation

Propertie:

Spectral Theorem

Othe

ODE Theor

Spectral Embedding

#### Spectrum and spectral radius

The spectrum of A is the set of eigenvalues of A. The spectral radius  $\rho(A)$  is the eigenvalue  $\lambda$  maximizing  $|\lambda|$ .

### Extending to $\mathbb{C}^{n\times n}$

Statistical Motivation

Properties

Spectral Theorem

Othe

ODE Theor

Spectral Embedding

### Complex conjugate

The complex conjugate of a number

$$z = a + bi \in \mathbb{C}$$
 is  $\overline{z} \equiv a - bi$ .

### Extending to $\mathbb{C}^{n\times n}$

Statistical Motivation

Propertie

Spectral Theorem

Othe

ODE Theor

Spectral Embedding

#### Complex conjugate

The complex conjugate of a number

$$z = a + bi \in \mathbb{C}$$
 is  $\overline{z} \equiv a - bi$ .

#### Complex transpose

The conjugate transpose of  $A \in \mathbb{C}^{m \times n}$  is

$$A^H \equiv \overline{A}^T$$
.

### Hermitian Matrix

Statistical Motivation

Properties

Spectral Theorem

Other

ODE Theor

$$A = A^H$$

Mathematics Methods for Computer Science

# Properties

Statistical Motivation

Propertie

Spectral Theorem

Other

**ODE Theor** 

Spectral Embedding

#### Lemma

All eigenvalues of Hermitian matrices are real.

### Properties

Statistical Motivation

Propertie

Spectral Theorem

Othe

ODE Theory

Spectral Embeddin

#### Lemma

All eigenvalues of Hermitian matrices are real.

#### Lemma

Eigenvectors corresponding to distinct eigenvalues of Hermitian matrices must be orthogonal.

## Spectral Theorem

Statistical Motivation

Propertie

Spectral Theorem

Othe

ODE Theory

Spectral Embedding

### Spectral Theorem

Suppose  $A \in \mathbb{C}^{n \times n}$  is Hermitian (if  $A \in \mathbb{R}^{n \times n}$ , suppose it is symmetric). Then, A has exactly n orthonormal eigenvectors  $\vec{x}_1, \dots, \vec{x}_n$  with (possibly repeated) eigenvalues  $\lambda_1, \dots, \lambda_n$ .

# Spectral Theorem

Statistical Motivation

Propertie

Spectral Theorem

Othe

ODE Theory

Spectral Embedding

### Spectral Theorem

Suppose  $A \in \mathbb{C}^{n \times n}$  is Hermitian (if  $A \in \mathbb{R}^{n \times n}$ , suppose it is symmetric). Then, A has exactly n orthonormal eigenvectors  $\vec{x}_1, \cdots, \vec{x}_n$  with (possibly repeated) eigenvalues  $\lambda_1, \cdots, \lambda_n$ .

Full set: 
$$D = X^T A X$$

### Matrix Inverse

Statistical Motivation

**Properties** 

Spectral Theorem

Other

ODE Theory

$$\vec{b} = c_1 \vec{x}_1 + \dots + c_k \vec{x}_k$$
$$A\vec{x} = \vec{b}$$

### Matrix Inverse

Statistical Motivation

**Properties** 

Spectral Theorem

Other

ODE Theory

$$\vec{b} = c_1 \vec{x}_1 + \dots + c_k \vec{x}_k$$
$$A\vec{x} = \vec{b}$$

$$\Rightarrow \vec{x} = \frac{c_1}{\lambda_1} \vec{x}_1 + \dots + \frac{c_n}{\lambda_n} \vec{x}_n$$

Statistical Motivation

**Properties** 

Spectral Theorer

Other

ODE Theory

$$\vec{b} = c_1 \vec{x}_1 + \dots + c_k \vec{x}_k$$
$$A\vec{x} = \vec{b}$$

$$\Rightarrow \vec{x} = \frac{c_1}{\lambda_1} \vec{x}_1 + \dots + \frac{c_n}{\lambda_n} \vec{x}_n$$

$$A = XDX^{-1} \Rightarrow A^{-1} = XD^{-1}X^{-1}$$

# Matrix Square Root

Statistical Motivation

Propertie

Spectral Theore

Other

ODE Theor

- $\bullet$  Given symmetric positive semi-definite (PSD) matrix, U
- ullet Can compute matrix square root,  $U^{1/2}$

# Application: Polar decomposition

- ullet Given real n-by-n matrix, A
- There exists a unique factorization called the Polar Decomposition

$$A = RU$$

where R is an n-by-n orthogonal matrix, and U is an n-by-n symmetric PSD right "stretch" matrix.

- Also a left stretch matrix, W, such that A = WR.
- Geometric interpretation.

Statistical Motivation

Propertie

Spectral Theore

Other

ODE Theor

# Application: Shape Matching

Statistical Motivation

Properties

Spectral Theore

Other

ODE Theo



- Fast Lattice Shape Matching (Fast LSM)
- SIGGRAPH 2007 [Rivers and James 2007]
- http://www.alecrivers.com/fastlsm
- Need to compute orientation, R, of local particle groups
- Millions of polar decompositions (and eigenvalue decomps) per second

# Physics (in one slide)

Statistical Motivation

Properties

Spectral Theorem

Othe

**ODE Theory** 

Spectral Embedding

# Newton:

$$\vec{F} = m \frac{d^2 \vec{x}}{dt^2}$$

# Physics (in one slide)

Statistical Motivation

**Properties** 

Spectral Theorem

Othei

**ODE Theory** 

Spectral Embedding

#### Newton:

$$\vec{F} = m \frac{d^2 \vec{x}}{dt^2}$$

#### Hooke:

$$\vec{F_s} = k(\vec{x} - \vec{y})$$

#### First-Order System

Statistical Motivation

Properties

Spectral Theorer

Othe

**ODE Theory** 

$$M\vec{X}'' = K\vec{X}$$

$$\longrightarrow \frac{d}{dt} \begin{pmatrix} \vec{X} \\ \vec{V} \end{pmatrix} = \begin{pmatrix} 0 & I_{3n \times 3n} \\ M^{-1}K & 0 \end{pmatrix} \begin{pmatrix} \vec{X} \\ \vec{V} \end{pmatrix}$$

#### General ODE

Statistical Motivation

Properties

Spectral Theoren

Other

**ODE Theory** 

$$\vec{Y}' = B\vec{Y}$$

# Eigenvector Solution

Statistical Motivation

**Properties** 

Spectral Theoren

Othe

**ODE Theory** 

$$\vec{y}' = B\vec{y}$$

$$B\vec{y}_i = \lambda_i \vec{y}_i$$

$$\vec{y}(0) = c_1 \vec{y}_1 + \dots + c_k \vec{y}_k$$

# Eigenvector Solution

Statistical Motivation

**Properties** 

Spectral Theorem

Othei

**ODE Theory** 

$$\vec{y}' = B\vec{y}$$

$$B\vec{y}_i = \lambda_i \vec{y}_i$$

$$\vec{y}(0) = c_1 \vec{y}_1 + \dots + c_k \vec{y}_k$$

$$\rightarrow \vec{y}(t) = c_1 e^{\lambda_1 t} \vec{y}_1 + \dots + c_k e^{\lambda_k t} \vec{y}_k$$

## Application: Modal Sound Synthesis

Statistical Motivation

Propertie:

Spectral Theorer

Othe

**ODE Theory** 

Spectral Embedding



Major role in physics-based sound synthesis https://www.youtube.com/watch?v=dMUHp8i6E5E

# Organizing a Collection

Statistical Motivation

Propertie

Spectral Theorem

Othe

ODE Theo



(a) Database of photos



(b) Spectral embedding

# Setup

Statistical Motivation

Propertie:

Spectral Theorer

Othei

ODE Theory

Spectral Embedding

**Have:** n items in a dataset

 $w_{ij} \geq 0$  similarity of items i and j

$$w_{ij} = w_{ji}$$

**Want:**  $x_i$  embedding on  $\mathbb{R}$ 

# Quadratic Energy

Statistical Motivation

Properties

Spectral Theorer

Othe

ODE Theory

$$E(\vec{x}) = \sum_{i,j} w_{ij} (x_i - x_j)^2$$

# Optimization

Statistical Motivation

**Properties** 

Spectral Theore

Other

ODE Theory

Spectral Embedding

 $\text{minimize } E(\vec{x})$ 

# Optimization

Statistical Motivation

**Properties** 

Spectral Theorer

Othe

ODE Theor

$$\begin{array}{c} \text{minimize } E(\vec{x}) \\ \text{such that } ||\vec{x}||_2^2 = 1 \end{array}$$

# Optimization

Statistical Motivation

**Properties** 

Spectral Theoren

Othei

ODE Theory

minimize 
$$E(\vec{x})$$
 such that  $||\vec{x}||_2^2 = 1$   $\vec{1}\vec{x} = 0$ 

## Simplification

Statistical Motivation

Propertie:

Spectral Theorem

Other

ODE Theory

$$E(\vec{x}) = 2\vec{x}^T (A - W)\vec{x}$$

Statistical Motivation

Properties

Spectral Theorem

Othe

ODE Theor

Spectral Embedding

Eigenvector of A - W with **second** smallest eigenvalue.