Mathematics Methods for Computer Science

Instructor: Xubo Yang

SJTU-SE DALAB

Lecture

Eigenproblems I:

$$A\vec{x} = \lambda\vec{x}$$

Setup

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

- Age
- Weight
- Blood pressure
- Heart rate

Setup

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

- Age
- Weight
- Blood pressure
- Heart rate

Find: Correlations between different dimensions

Simplest Model

One-dimensional subspace

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

Simplest Model

One-dimensional subspace

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

Equivalently:

$\vec{x}_i \approx c_i \hat{v}$ (进行线性拟合)

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

Variational Idea

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

$$\text{such that } ||\hat{v}||_2 = 1$$

Variational Idea

这个等价问题说的是，求出每个数据点相对于拟合曲线的偏置量的和的最小值，此最小值对应于拟合精度最高的v

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

What does the constraint do?

Variational Idea

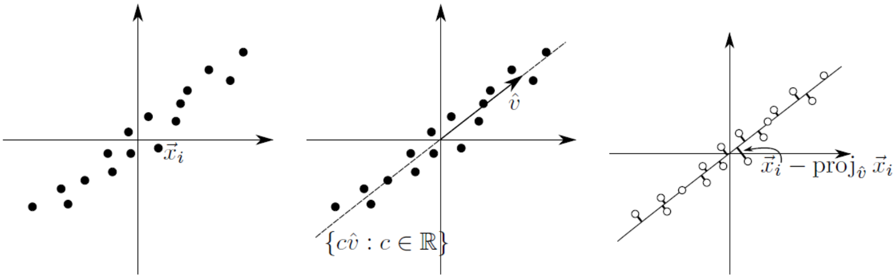
$$\mathit{minimize}_{\hat{v}} \sum_i ||\vec{x}_i - \mathit{proj}_{\hat{v}} \vec{x}_i||_2^2$$
$$\text{such that } ||\hat{v}||_2 = 1$$

What does the constraint do?

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

(无需在除去v模长)

Geometric Interpretation



(a) Input data (b) Principal axis (c) Projection error

Review from Last Lecture

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

What is c_i ?

Review from Last Lecture

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

垂直的时候最短！
，由于|v|=1，故c
就是投影长度

What is c_i ?

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

Equivalent Optimization

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

X^T*v可以理解为：所有点x_i在v向量方向上的投影构成的列向量

End Goal

Eigenvector of XX^T with largest eigenvalue.

Gram矩阵

End Goal

Eigenvector of XX^T with largest eigenvalue.

"First principal component"

More after SVD!

Definitions

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 $\lambda \in \mathbb{R}$; λ is an eigenvalue. Complex eigenvalues and eigenvectors instead have $\lambda \in \mathbb{C}$ and $\vec{x} \in \mathbb{C}^n$.

Definitions

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 $\lambda \in \mathbb{R}$; λ 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

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

Eigenproblems in the Wild

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

ODE:常微分方程
PDE:偏微分方程

Eigenproblems in the Wild

- Optimize $||A\vec{x}||_2$ such that $||\vec{x}||_2 = 1$ (important!)
- ODE/PDE problems: Closed solutions and approximations for $\vec{y}' = B\vec{y}$
- Critical points of Rayleigh quotient:
$$\frac{\vec{x}^T A\vec{x}}{||\vec{x}||_2^2}$$

Two Basic Properties

Proved in textbook

Lemma

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

Two Basic Properties

Proved in textbook

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

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

nondefective：无瑕疵的，diagonalizble：可对角化的

Nondefective

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

这个定理说的是，n维矩阵A如果有n个线性无关的特征向量，则称A是可对角化的。

Diagonalizability

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

(矩阵A的谱)

Spectrum and spectral radius

The spectrum of A is the set of eigenvalues of A.

The spectral radius $\rho(A)$ is the eigenvalue λ maximizing $|\lambda|$.

(矩阵A的谱半径)

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

Complex conjugate

The complex conjugate of a number $z = a + bi \in \mathbb{C}$ is $\bar{z} \equiv a - bi$.

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

Complex conjugate

The complex conjugate of a number $z = a + bi \in \mathbb{C}$ is $\bar{z} \equiv a - bi$.

Complex transpose

The conjugate transpose of $A \in \mathbb{C}^{m\times n}$ is $A^H \equiv \bar{A}^T$.

(A的共轭矩阵的转置)

Hermitian Matrix

(哈密顿矩阵)

$$A = A^H$$

Properties

Lemma

All eigenvalues of Hermitian matrices are real.

Properties

Lemma

All eigenvalues of Hermitian matrices are real.

Lemma

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

Spectral Theorem

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 $\lambda_1, \cdots, \lambda_n$.

Spectral Theorem

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

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

Matrix Inverse

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

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

Matrix Inverse

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

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

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

Matrix Square Root

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

Application: Polar decomposition

- 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.

Application: Shape Matching

- 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)

Newton:

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

Physics (in one slide)

Newton:

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

Hooke:

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

First-Order System

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

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

General ODE

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

Eigenvector Solution

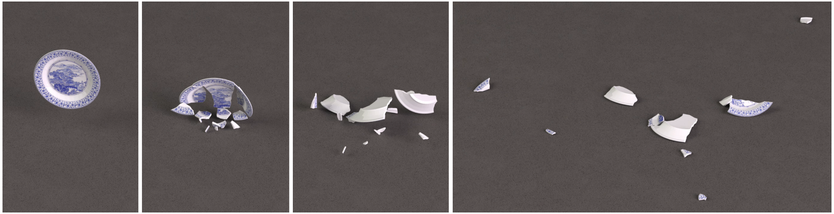
$$\vec{y}' = B\vec{y}$$
$$B\vec{y}_i = \lambda_i \vec{y}_i$$
$$\vec{y}(0) = c_1\vec{y}_1 + \cdots + c_k\vec{y}_k$$

Eigenvector Solution

$$\vec{y}\,' = B\vec{y}$$
$$B\vec{y}_i = \lambda_i \vec{y}_i$$
$$\vec{y}(0) = c_1\vec{y}_1 + \cdots + c_k\vec{y}_k$$

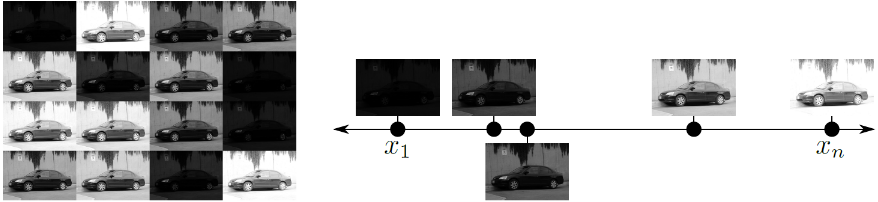
$$\rightarrow \vec{y}(t) = c_1 e^{\lambda_1 t}\vec{y}_1 + \cdots + c_k e^{\lambda_k t}\vec{y}_k$$

Application: Modal Sound Synthesis



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

Organizing a Collection



(a) Database of photos (b) Spectral embedding

Setup

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

$$E(\vec{x}) = \sum_{ij} w_{ij} \left(x_i - x_j\right)^2$$

Optimization

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

Optimization

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

Optimization

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

Simplification

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

Desired

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