CS5284 : Graph Machine Learning

Lecture 2 : Introduction to Graph Science

Semester 1 2024/25

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Course lectures

- Introduction to Graph Machine Learning
- Part 1: GML without feature learning (before 2014)
  - Introduction to Graph Science
  - Graph Analysis Techniques without Feature Learning
    - Graph clustering
    - Graph SVM
    - Recommendation on graphs
    - Graph-based visualization
- Part 2 : GML with shallow feature learning (2014-2016)
  - Shallow graph feature learning
- Part 3 : GML with deep feature learning, a.k.a. GNNs (after 2016)
  - Graph Convolutional Networks (spectral and spatial)
  - Weisfeiler-Lehman GNNs
  - Graph Transformer & Graph ViT
  - Graph generation & molecular science
  - GNNs for combinatorial optimization
  - Integrating GNNs and LLMs
  - Benchmarking GNNs
  - GNNs for recommendation & knowledge graphs

Outline

- Graph theory
- Graph categories
- Basic definitions
- Curse of dimensionality and structure
- Manifolds and graphs
- Spectral graph theory
- Graph construction
- Conclusion

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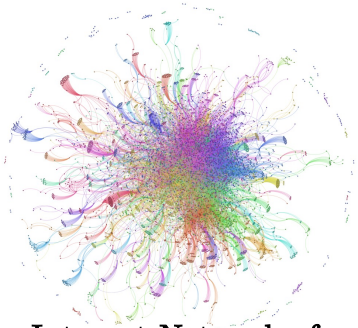
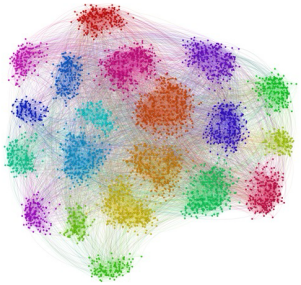
Graphs

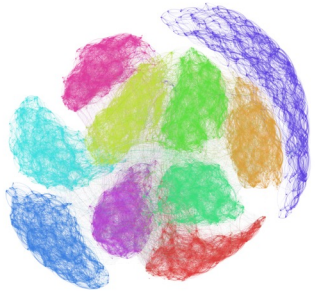
- Graphs encode complex data structures.
  - They are everywhere! Internet, social networks, customer-product relationships, etc



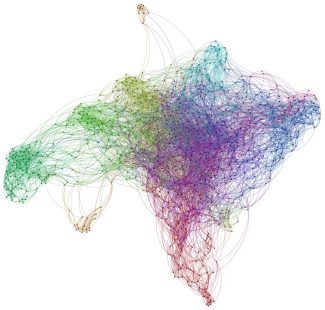
Internet Network of California



Social Network

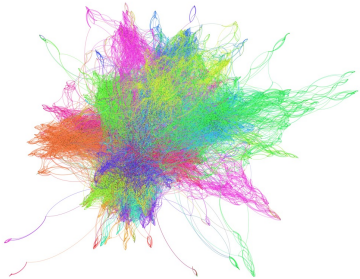


MNIST Image Network



GTZAN Music Network

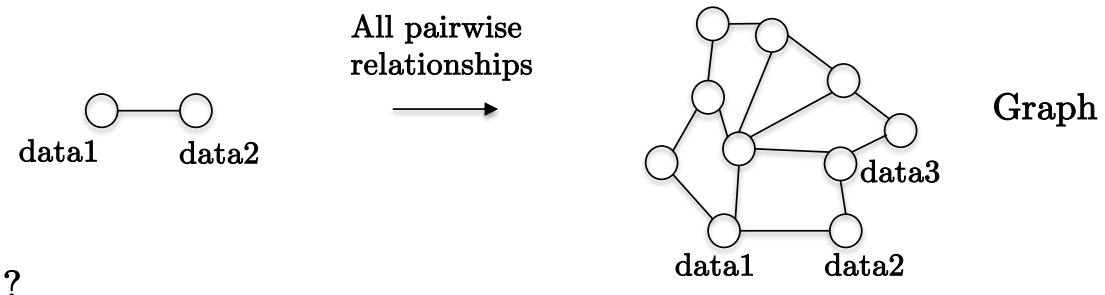
- "Graphs are the most important discrete models in the world." - Gil Strang (MIT)



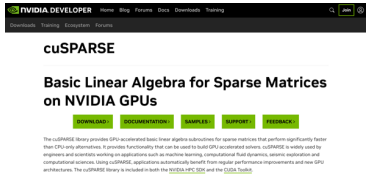
Network of Text Documents 20newsgroups

Graphs

- Definition : (Simple) mathematical model representing pairwise relationships between data.

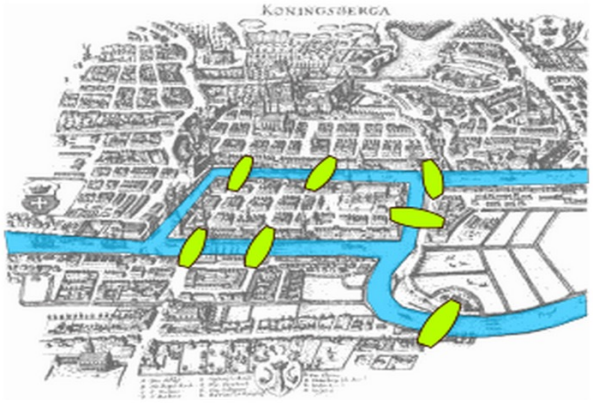


- Why are graphs useful?
  - Graphs offer a global view and analysis of data structures.
    - They possess meaningful patterns, i.e. insights about data properties.
  - Some tasks are exclusively designed for graphs, e.g. Google PageRank recommendation.
  - They can boost performance with additional priors, a.k.a. inductive bias.
  - They can benefit from GPUs as graphs are (sparse) matrices.



Graph theory

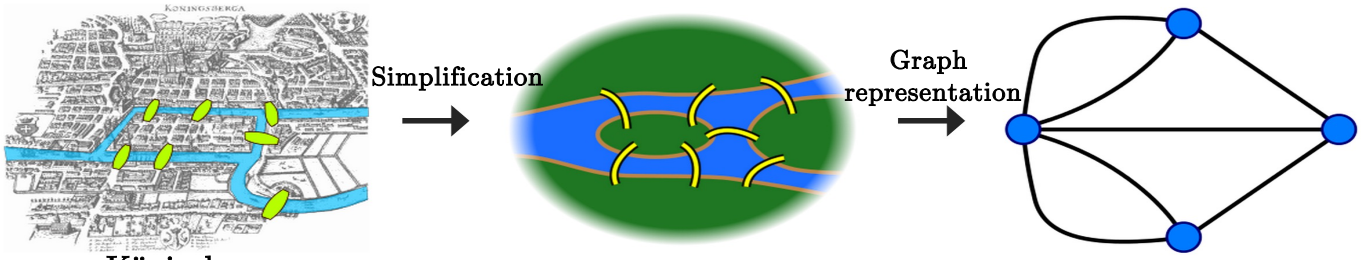
- When did it start?
  - History of graph theory : Graphs have been formally studied since 1736, starting with Mathematician Leonhard Euler and the famous problem of "Seven Bridges of Königsberg" :



Königsberg
City

In-lecture question

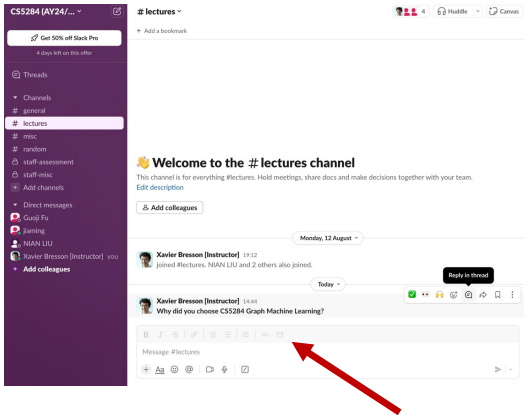
- Can we find a path through the city (starting from any place) that crosses each bridge once and only once? Justify your response.



Königsberg City

Source: Wikipedia.

- In Slack #lectures
  - Identify the question and Reply in thread with a short response



Graph theory

- When did it start?
  - History of graph theory : Graphs have been formally studied since 1736, starting with Mathematician Leonhard Euler and the famous problem of “Seven Bridges of Königsberg” :

- Graph theory have since developed tools to analyze and process networks for all sort of applications : clustering, classification, visualization, recommendation, etc.

Outline

- Graph theory
- **Graph categories**
- Basic definitions
- Curse of dimensionality and structure
- Manifolds and graphs
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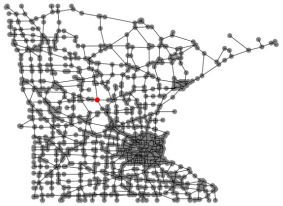
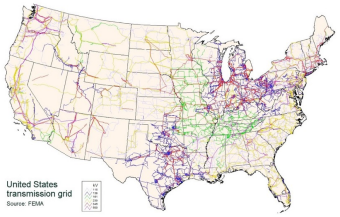
Graph categories

- Natural Graphs
  - Social networks : Meta, LinkedIn, Twitter
  - Biological networks : Brain connectivity & functionality, gene regulatory networks
  - Communication networks : Internet, networking devices
  - Transportation networks : Trains, cars, airplanes, pedestrians
  - Power networks : Electricity, water
- Natural graphs mean graphs that are not artificially hand-crafted/constructed.



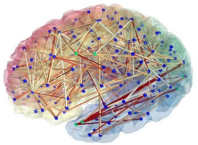
Minnesota Road Network

Telecommunication Network



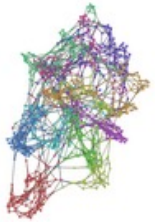
US Electrical Network

Facebook



Brain Connectivity

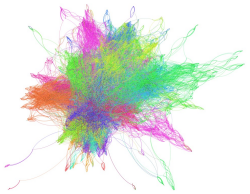
=



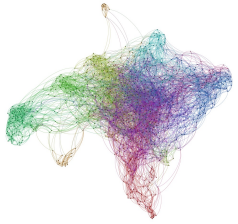
Graphs

Graph categories

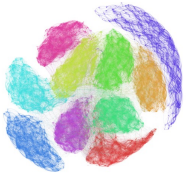
- Graphs constructed from data :
  - MNIST image network
  - GTZAN music network
  - 20NEWS text document network
  - 3D mesh points



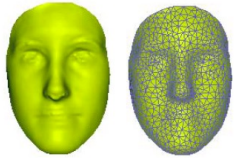
Graph of Text Documents
20newsgroups



GTZAN Music Graph



MNIST Image Graph



3D mesh points

- Optimal graph construction : Unfortunately, no theoretical approach is available – it is empiricial and depends mostly on domain expertise knowledge and good common practice (later discussed).

- What is the computational time needed to construct a graph from data features ?
  - Exact construction : $O(n^2.d)$, n = num data, d = num features.

    for d = 1K, n = 1K ⇒ time < 1sec

    n = 100K ⇒ time = 1 min

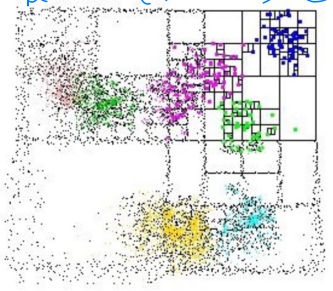
    n = 1M ⇒ time > 1 hour

  - Approximate technique : kd-trees O(nlogn.d) with e.g. FLANN[1], a library for fast approximate nearest neighbor search in high-dimensional spaces.

edge features ba. If node features, should be $O(n^2 + dn)$

n^2 : Going through adjacency matrix A of size n^2.

d : Adding of d features per edge

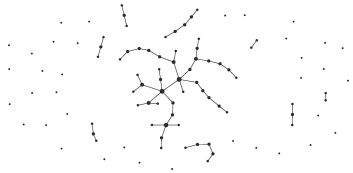


[1] https://github.com/flann-lib/flann

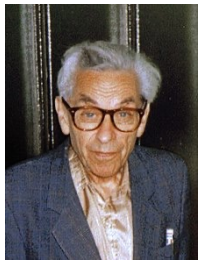
Graph categories

- Mathematical/simulated graphs
  - Erdos-Renyi graphs[1]
  - Stochastic block models (SBM)[2]
  - Lancichinetti-Fortunato-Radicchi (LFR) graphs[3]

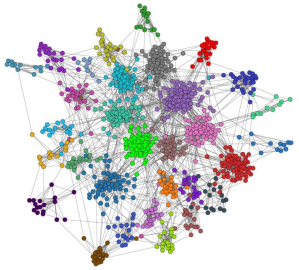
Graphs generated by some random process



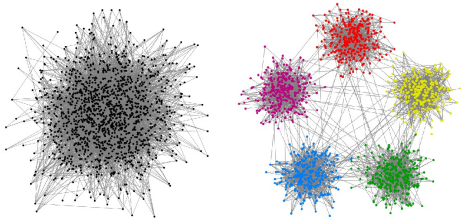
Erdos-Renyi Network
Source: Wikipedia.



Paul Erdős
1913 – 1996



LFR
Source: Kojaku, 2018



SBM
Source: Abbe, JMLR'17

- Why using artificial networks?
  - Mathematical Modeling
    - Advantage : Precise control of your data model (estimate best performance given some data assumptions). No need to perform extensive experiments.
    - Limitation : Most data assumptions are often too restrictive, and it is not guaranteed that real-world data follow the given model assumptions.

can find out some graph properties given it follows certain assumptions

[1] Erdos, Renyi, On random graph, 1959
[2] Anderson, Wasserman, Faust, Building stochastic blockmodels, 1992
[3] Lancichinetti, Fortunato, Filippo, Benchmark graphs for testing community detection algorithms, 2008

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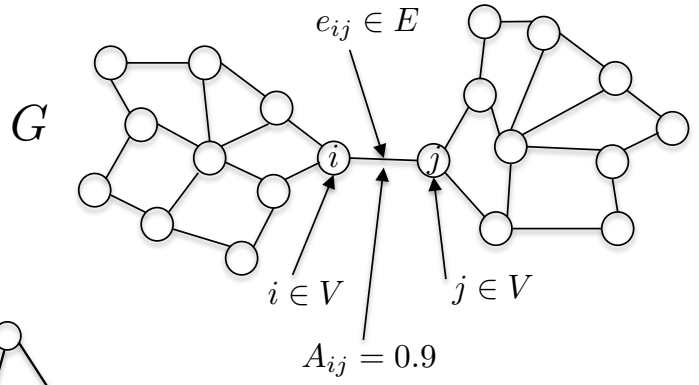
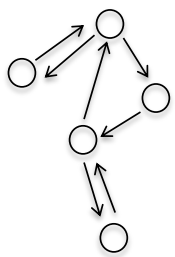
Basic definitions

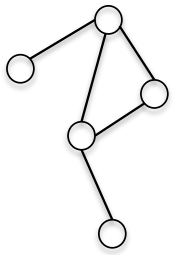
- Graphs are defined as G = (V,E,A) where
  - V is the set of vertices (or nodes) w/ |V| = n.
  - E is the set of edges.
  - A is the adjacency similarity matrix.



- Directed or undirected graphs :

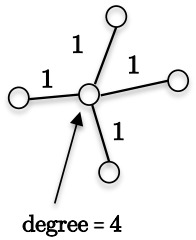


Directed graph

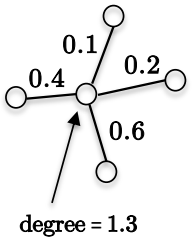


Undirected graph

- Node degree :
  - For binary graphs, $A_{ij} = \{0,1\}$ ⇒ degree = num of edges connected to a node
  - For weighted graphs, A_{ij} in [0,1] ⇒ degree is defined as $d_i = \sum_{j \in V} Aij$



Binary graph

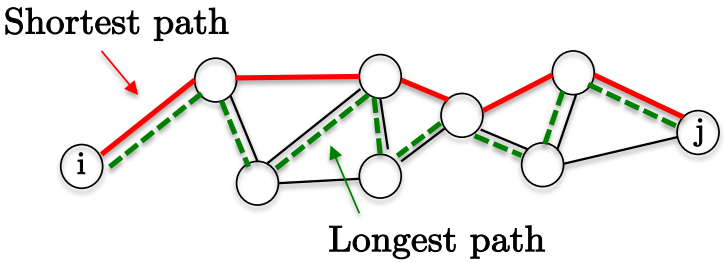


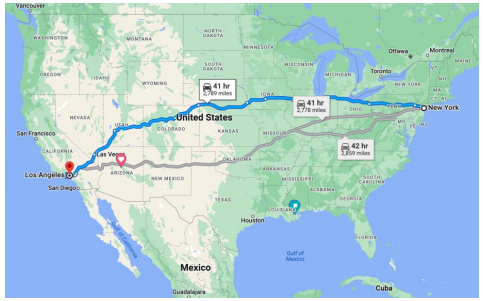
Weighted graph

Degree in both binary and weighted graphs = $d_i = \sum_{j \in V} A_{ij}$

Algorithms

- Standard graph algorithms (a.k.a. software engineering, no learning) :
  - Breadth-first search, depth-first search, minimum spanning tree, topological sorting, strongly connected components, graph colouring, maximum flow/minimum cut, graph matching, etc.
- Shortest path algorithm : Find a path on a graph with the smallest possible length.
  - Fast Algorithm : Dijkstra's algorithm[1]
  - Popular application is the road navigator product, e.g. from New York to Los Angeles.



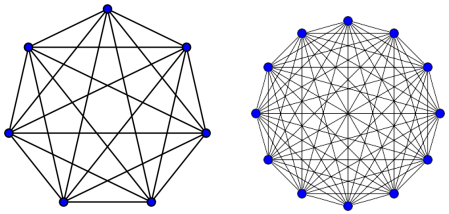


[1] Dijkstra, A note on two problems in connexion with graphs, 1959

Dense vs. sparse graphs

- Dense/complete/full graphs : Each vertex is connected to all other vertices.

$$|E| = \frac{n(n-1)}{2} = O(n^2)$$

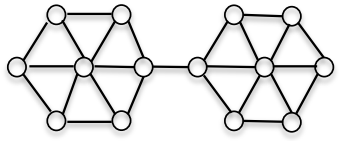


Dense graphs

- Sparse graphs : Each vertex is connected to a few other k≪n vertices.

$$|E| = O(kn) = O(n)$$

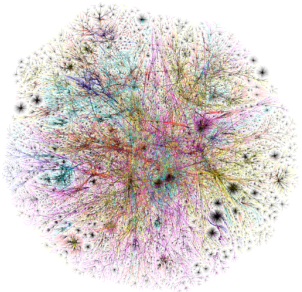
$k = E(deg(v)) = constant$!!



Sparse graph

- Which graph is better -- dense or sparse?
  - Sparse networks are highly desirable for memory and computational efficiency.
    For instance, Internet has n = 4.73 billion pages (as of August 2016)
    - $|E| = n^2 = 10^{18}$ if Internet was full.
    - $|E| = k.n = 10^{11}$ as it is sparse with $k \approx 100$ (mean degree).

Each page references about 100 other pages



Internet

- Actually, most real-world networks (e.g. social, communication, etc) are sparse !
  - Because sparsity induces structure (a fully connected graph has no structure).

goooood

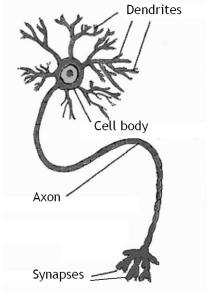
the relationships between nodes gives no information / value

In-lecture question

- In the human brain, some 86 billion neurons form 100 trillion axon connections to each other. Can we model the human brain as a sparse graph? What is the percentage of non-zero elements?
  - n = ? $86 \times 10^9 = 8.6 \times 10^{10}$
  - |E| = ? $100 \times 10^{12} = 10^{14}$

$$\text{mean degree} = \frac{10^{14}}{8.6 \times 10^{10}} = 86000$$ ← sparse in comparison to 8.6×10^9 nodes

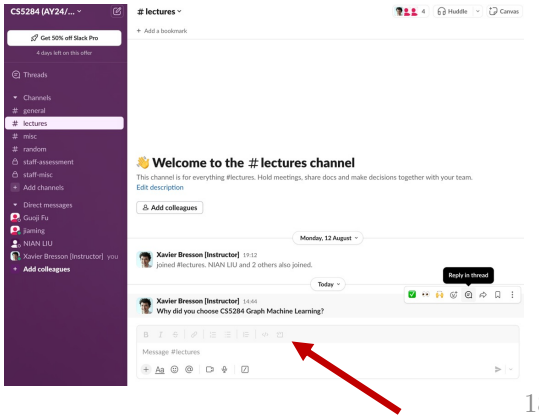
$$\% \text{ of Non-zero elements in the adjacency matrix} = \frac{86000}{8.6 \times 10^9} \times 100\% = \left[\frac{8.6 \times 10^4}{8.6 \times 10^9} \times 100\right]\% = 10^{-3}\%$$



One neuron
Inputs are dentrites
Outputs are synapses
Connections are axons

Human biological neural network

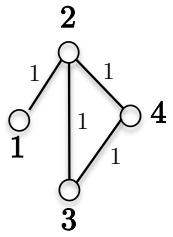
- In Slack #lectures
  - Identify the question and Reply in thread with a short response



Adjacency matrix

- **Definition : Matrix A in G = (V,E,A) represents structural/topological information about the network. We have two classes of A :**
  - **Binary matrix : $A_{ij} \in \{0,1\}$**

$$A_{ij} = \begin{cases} 1 \text{ if } (i,j) \in E \\ 0 \text{ otherwise} \end{cases}$$

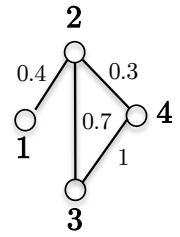
G = 

$$\Rightarrow A = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \end{array} \begin{array}{c} \begin{array}{cccc} 1 & 2 & 3 & 4 \end{array} \\ \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix} \end{array}$$

  - **Weighted matrix : $A_{ij} \in [0,1]$ (commonly normalized to 1)**

How is this normalization done?

$$A_{ij} = \begin{cases} \in [0,1] \text{ if } (i,j) \in E \\ 0 \text{ otherwise} \end{cases}$$

G = 

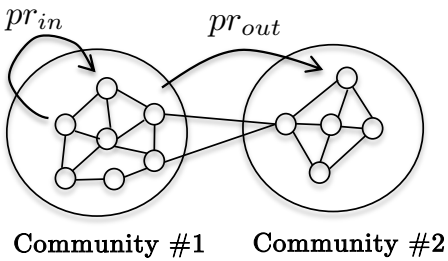
$$\Rightarrow A = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \end{array} \begin{array}{c} \begin{array}{cccc} 1 & 2 & 3 & 4 \end{array} \\ \begin{bmatrix} 0 & 0.4 & 0 & 0 \\ 0.4 & 0 & 0.7 & 0.3 \\ 0 & 0.7 & 0 & 1 \\ 0 & 0.3 & 1 & 0 \end{bmatrix} \end{array}$$

not normalized?

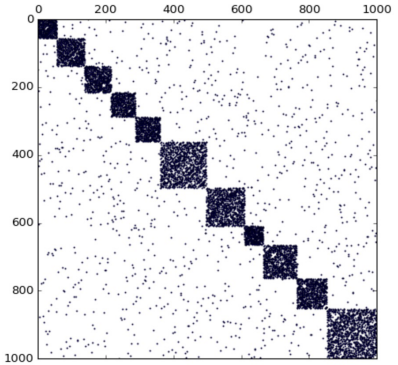
Lab 1 : LFR social networks

- Run code01.ipynb and synthesize LFR social networks.
  - Play with the mixing parameter μ :
    - μ small : Communities are well separated.
    - μ large : Communities are mixed.

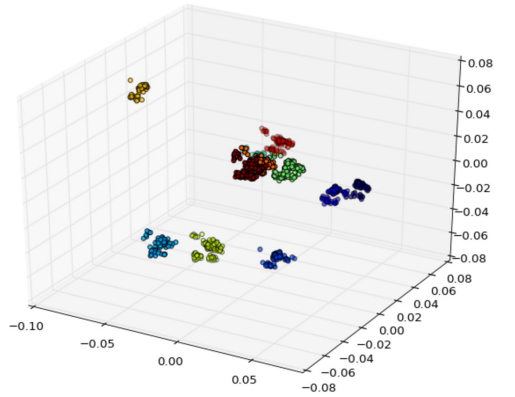
$$\mu = \frac{pr_{out}}{pr_{in}}$$




```
In [15]: # Plot same W but according to communities
         # Any structure?
         plt.figure(2)
         plt.spy(W,precision=0.01, markersize=1)
         plt.show()
```




```
In [19]: # Visualize the social network in 3D
         fig = pylab.figure(4)
         ax = Axes3D(fig)
         ax.scatter(X, Y, Z, c=C)
         pyplot.show()
```

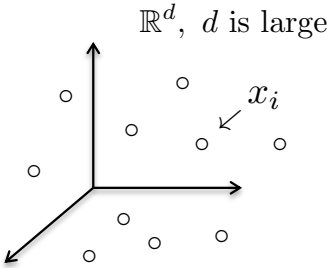


Outline

- Graph theory
- Graph categories
- Basic definitions
- **Curse of dimensionality and structure**
- Manifolds and graphs
- Spectral graph theory
- Graph construction
- Conclusion

Curse of dimensionality

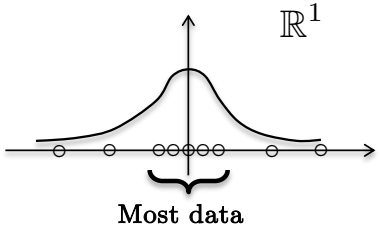
- What is the curse of dimensionality ?
  - In high dimensions, Euclidean distance between data becomes meaningless.
  - Theorem[1] : Suppose data are uniformly distributed in R^{d}, pick any data $\mathrm{x_i} \in \mathrm{V}$, we have :



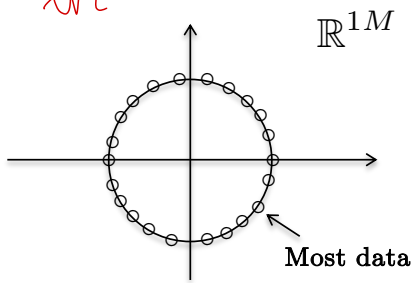
$$\lim_{d \to \infty} \mathbb{E}_{x_i}\left(\frac{\mathrm{d}^{\ell_2}_{\max}(x_i, V \setminus x_i) - \mathrm{d}^{\ell_2}_{\min}(x_i, V \setminus x_i)}{\mathrm{d}^{\ell_2}_{\min}(x_i, V \setminus x_i)}\right) = 0$$

Interpretation : All data are far away to each other with the same distance value !

- Besides, loss of intuition in high dimensions, e.g. with the Normal distribution :
  - In low-dim, most data are concentrated at the center.
  - In high-dim, most data are concentrated on the surface.



1-D Gaussian

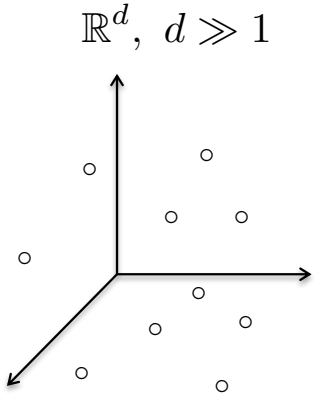


1,000,000-D Gaussian

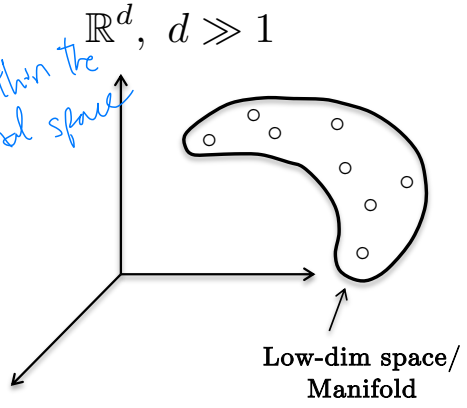
[1] Beyer, Goldstein, Ramakrishnan, Shaft, When is "nearest neighbor" meaningful? 1999

Blessing of structure

- What is the blessing of structure ?
  - Previously, the assumption "data are uniformly" distributed is actually not true for real-world data. Data have always properties, i.e. structures or invariances, such that they belong to a low-dimensional space called manifold where (geodesic) distances are meaningful.



Uniform distribution of data
No structure/randomness



Non-Uniform distribution of data
Structure/inductive bias

Outline

- Graph theory
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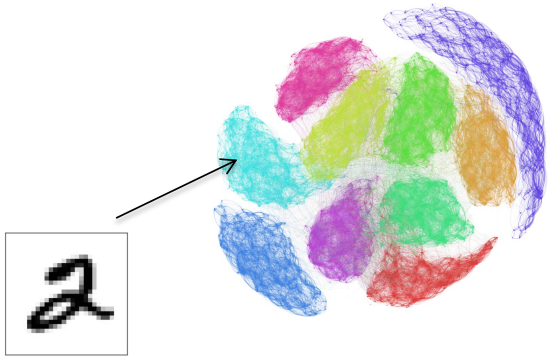
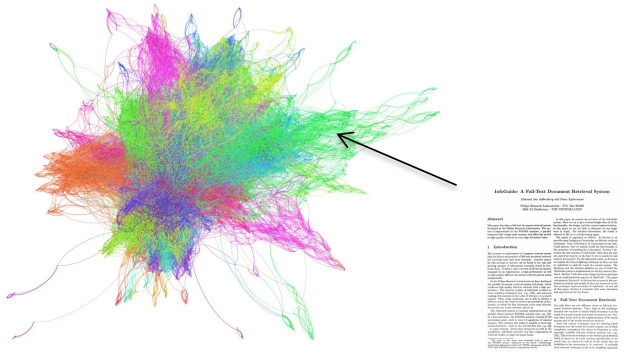
Manifold learning

- It can be challenging to identify structures hidden in data because of
  - The curse of dimensionality (i.e. high-dimensional data).
  - Some data have easy structures, but most have complex ones.
- A class of algorithms that extracts low-dimensional patterns is manifold learning (later discussed).



MNIST Image Graph

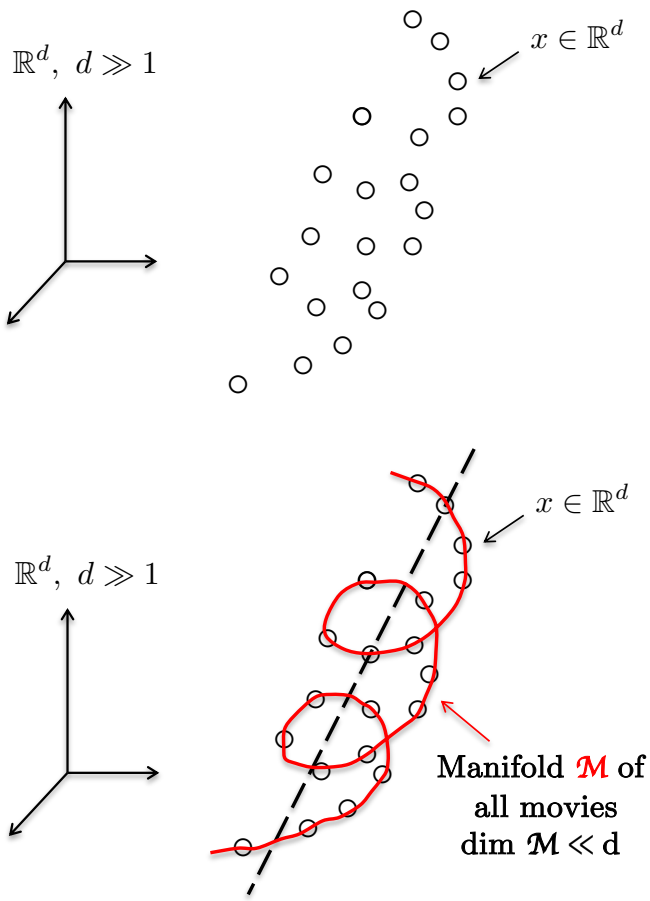


Graph of Text Documents 20newsgroups

From manifolds to graphs

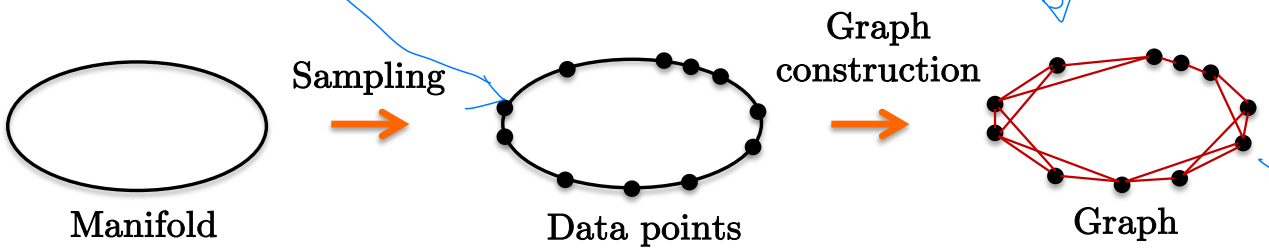
- Manifold assumption : High-dimensional data are sampled from a low-dimensional manifold.
  - Example : Let x be a movie, each movie is defined by d features/attributes like genre, actors, release year, origin country, etc such that x in R^d. We can make the assumption that all movies form a manifold $\mathcal{M}$ in R^d.

- Assumption validity : The manifold is a good working hypothesis for
  - Several types of data, including images, text documents, music, etc.
  - Most machine learning tasks e.g. classification, visualization, recommendation.
  - However, it can also be limited as it can be a crude approximation of the (true) data distribution.



From manifolds to graphs

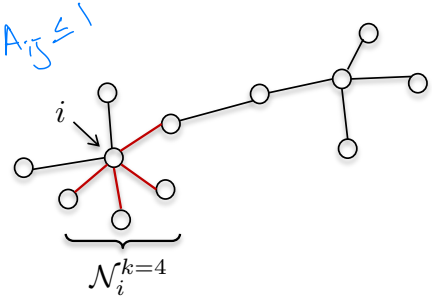
- **Graphs can be regarded as a manifold sampling process.**
  - The manifold information is represented by a neighborhood graph (observe that the manifold is never directly observed or constructed).



- Neighborhood graphs :
  - Most populars are **k-NN graphs** defined as :

$$A_{ij} = \begin{cases} e^{-\frac{\text{dist}(x_i,x_j)^2}{\sigma^2}} & \text{if } j \in \mathcal{N}_i^k \\ 0 \text{ otherwise} \end{cases}$$

where $\text{dist}(x_i,x_j)$ is a distance (to be decided) between x_i and x_j, σ is the scale parameter (value depends on the dataset), and $\mathcal{N}_i^k$ is the neighborhood of data x_i.



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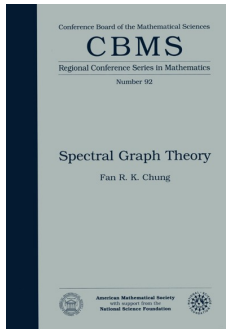
Spectral graph theory

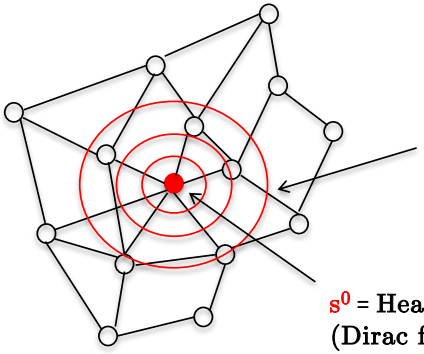


Fan Chung
SGT book
1997

- Given a graph G = (V,E,A), spectral graph theory (SGT) can
  - Find meaningful patterns that reveal multi-scale graph structures.
  - Process data defined on the graph domain (a.k.a. graph signal processing).
  - Boost performance of learning tasks s.a. clustering, classification, recommendation, etc.

- The most fundamental tool in SGT is the graph Laplacian operator L.
  - Why is the Laplacian useful?
    - It is the central operator of diffusion processes (on graphs).
    - Basis functions of this operator are the well-known Fourier modes (later discussed).

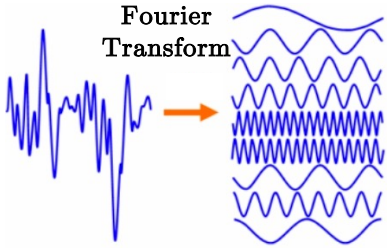
Pierre-Simon Laplace
(1749–1827)



Heat propagation using Laplacian operator :

$$s^{t+1} = Ls^t$$

s^0 = Heat source (Dirac function)



Graph Laplacian

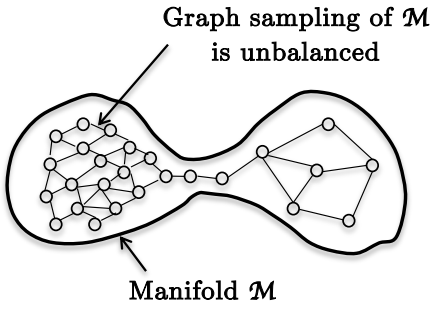
- **Un-normalized/combinatorial graph Laplacian :**

$$\underset{n \times n}{L_{un}} = D - A \quad \text{with D is the degree matrix :} \quad D = \text{diag}(d_1, ..., d_n),$$

$$n = |V| \qquad d_i = \sum_j A_{ij}$$

- Normalized Laplacian (most popular) :
  - Robust w.r.t. unbalanced sampling

$$L = D^{-1/2} L_{un} D^{-1/2} = I_n - D^{-1/2} A \; D^{-1/2}$$



- Random Walk Laplacian (for Google PageRank, later discussed) :

$$L = D^{-1} L_{un} = I_n - D^{-1} A$$

- All Laplacians are diffusion operators.

Graph spectrum

- Spectral graph theory can extract the modes of variation of the graph system.
  - How? With the eigenvalue decomposition (EVD) of the Laplacian operator L :

$$L = U\Lambda U^T \in \mathbb{R}^{n\times n} \text{ with}$$

$$U = [u_1, ..., u_n] \in \mathbb{R}^{n\times n},$$

$$U^T U = I_n, \text{ i.e. } \langle u_k, u_{k'} \rangle = \begin{cases} 1 & k = k' \\ 0 & \text{otherwise} \end{cases},$$

$$\Lambda = \text{diag}(\lambda_1, ..., \lambda_n) \in \mathbb{R}^{n\times n},$$

$$0 = \lambda_{\min} = \lambda_1 \leq \lambda_2 \leq ... \leq \lambda_n \leq 2$$

  - Interpretation:
    - u_k : Laplacian eigenvectors a.k.a. Fourier functions, i.e. vibration modes of the graph.
    - λ_k : Laplacian eigenvalues a.k.a. frequencies of the Fourier functions, i.e. how fast u_k vibrate.
  - EVD answers the famous question 'Can One Hear the Shape of a Drum'?[1]

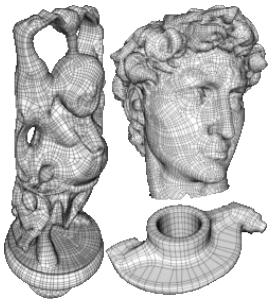
[1] Kac, Can One Hear the Shape of a Drum, 1966

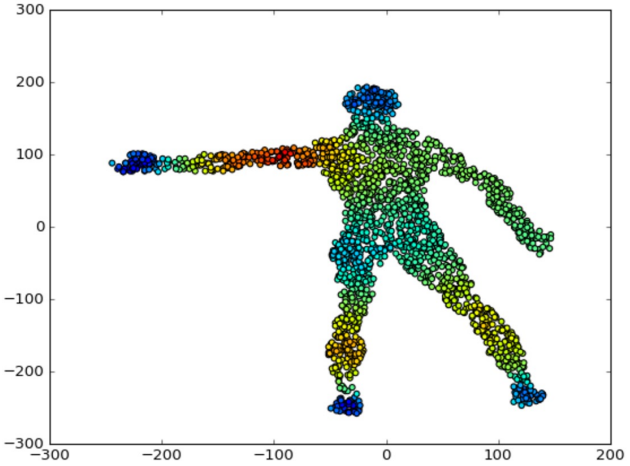
Lab 2 : Spectrum of point cloud and grid

- Run code02.ipynb and visualize the Fourier functions of a human body graph and a regular grid.
- What is the main property of the smallest and largest eigenvectors?
  - Smallest eigenvectors ⇒ Smoothest modes of vibration, i.e. low-frequency information. Global information
  - Largest eigenvectors ⇒ Highest frequencies of the graph, i.e. details or noise. Local information

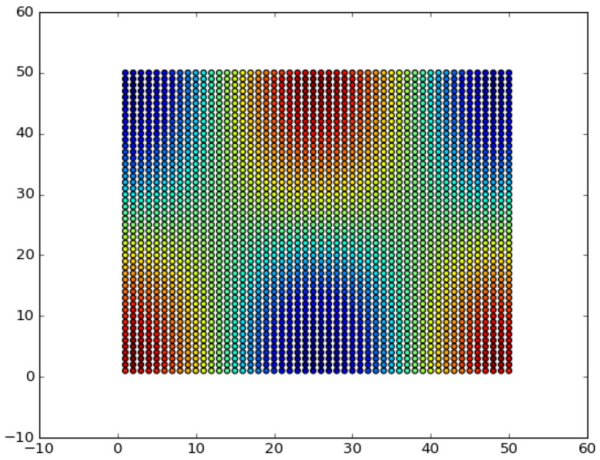
```
In [5]:
# Compute graph Laplacian
L = graph_laplacian(W)

# Compute modes of variations of graph system = Fourier functions
lamb, U = scipy.sparse.linalg.eigsh(L, k=9, which='SM')
```



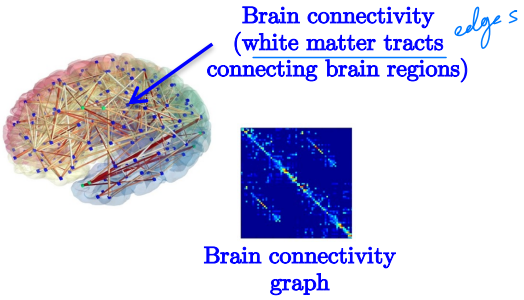


Fourier mode from a Graph =
Set of points or meshes in graphics
(e.g. 2D/3D shape recognition)

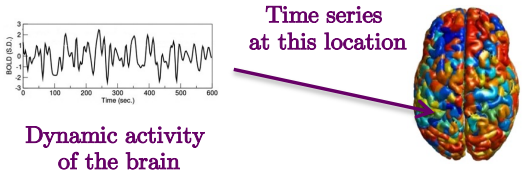


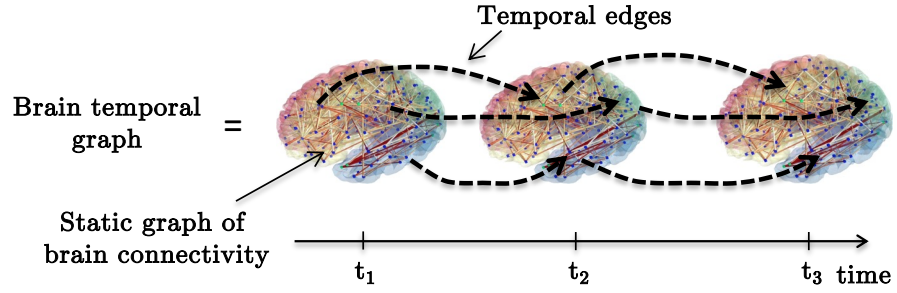
Fourier mode from a Graph =
Regular grid
(e.g. JPEG image compression,
most used technique)

Spectrum of human brain

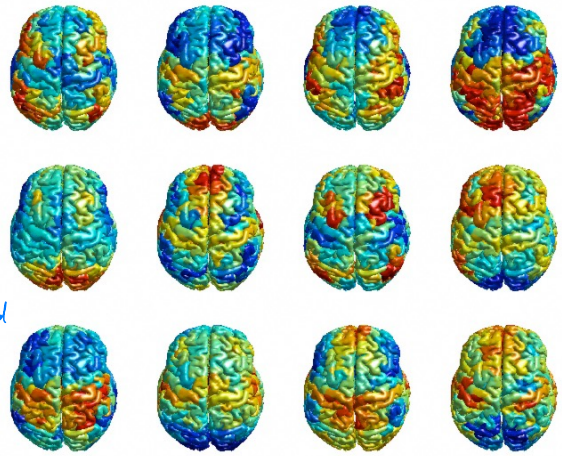


- Goal : Find brain activation patterns from structural MRI, a.k.a. brain resting states (brain structure implies brain function).
- Methodology : Given G (brain connectivity graph) ⇒ design a temporal graph ⇒ compute Laplacian L ⇒ compute eigenvectors u_k ⇒ visualize brain temporal activation patterns.
- Result : u_k represent the dynamic patterns related to basic functional brain tasks s.a. vision, body motor, language, etc.
- How to construct the brain temporal graph?





⇒ Result is 1 huge graph consisting of nodes connected by BOTH temporal edges and edges formed by the white matter tracts



Laplacian eigenvectors u_k
a.k.a. brain resting states
(video)

Spectral Graph Theory

$L = D - A$

$D = \text{diag}(\deg(v_1), \deg(v_2), \ldots, \deg(v_N))$

$A = \text{Binary } (N \times N) \text{ matrix}$

$$x^T L x = \sum_i^N \sum_j^N L_{ij} x_i x_j$$

$$L_{ij} x_i x_j = \begin{cases} \text{diag}(v_i) x_i^2 & \text{if } i = j \\ -E(v_i, v_j) x_i x_j & \text{otherwise} \end{cases}$$

$$x^T L x = \sum_i^N \text{diag}(v_i) x_i^2 - \sum_i^N \sum_j^N E(v_i, v_j) x_i x_j$$

$$\begin{pmatrix} x_1 & x_2 & x_3 \end{pmatrix} \begin{pmatrix} L_{11} & L_{12} & L_{13} \\ L_{21} & L_{22} & L_{23} \\ L_{31} & L_{32} & L_{33} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} x_1 & x_2 & x_3 \end{pmatrix} \begin{pmatrix} L_{11}x_1 + L_{12}x_2 + L_{13}x_3 \\ L_{21}x_1 + L_{22}x_2 + L_{23}x_3 \\ L_{31}x_1 + L_{32}x_2 + L_{33}x_3 \end{pmatrix}$$

$$= L_{11}x_1^2 + L_{12}x_1x_2 + L_{13}x_1x_3 + L_{21}x_1x_2 + L_{22}x_2^2 + L_{23}x_2x_3 + L_{31}x_1x_3 + L_{32}x_2x_3 + L_{33}x_3^2$$

$$= \sum_i^d \sum_j^d L_{ij} x_i x_j$$

Outline

Qn: Is it possible to reconstruct a graph solely using data about each node's degree?

Ans: No.

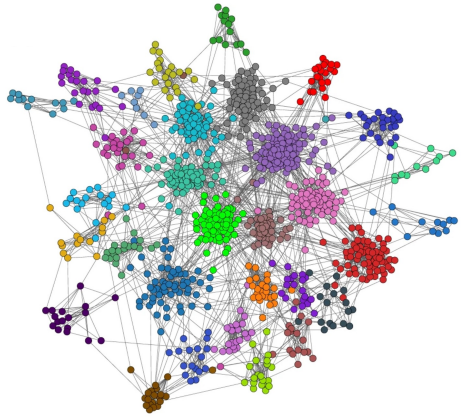
i	$\deg(v_i)$
1	2
2	2
3	2
4	1
5	1

This can be two different graphs

This is why we need either set E or matrix A

How to construct graphs from data?

- Three basic questions
  - Which type of graphs?
  - Which data distance?
  - Which data feature?



- Optimal graph construction
  - No universal recipe is available (no theory).
  - It depends on data and analysis task (empirical).
  - Domain expertise and good practice are essential.

Type of constructed graphs

complexity to construct : $O(kN)$

- Neighborhood graphs
  - k-NN graphs, i.e. sparse graphs by design.
  - Parameters
    - k : number of nearest neighbors, a common value is between {5,50}.
    - σ : positive scale parameter
- Two options to compute scale σ
  - Global scale : σ = mean distance of all k^{th} neighbors.
  - Local scale[1] : σ_i = distance of the k^{th} nearest neighbor for node i. (most common)

Same scaling hyperparameter to apply to all nodes

$$A_{ij} = \begin{cases} e^{-\frac{\text{dist}(x_i,x_j)^2}{\sigma^2}} & \text{if } j \in \mathcal{N}_i^k \\ 0 \text{ otherwise} \end{cases}$$

Adjacency matrix with global scale

sensitive to outliers.

$$A_{ij} = \begin{cases} e^{-\frac{\text{dist}(x_i,x_j)^2}{\sigma_i \sigma_j}} & \text{if } j \in \mathcal{N}_i^k \\ 0 \text{ otherwise} \end{cases}$$

Adjacency matrix with local scale

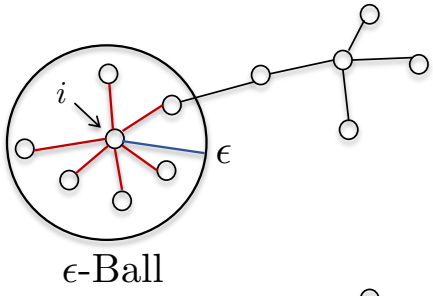
[1] Zelnik-Manor, Perona, Self-tuning spectral clustering, 2004

In-lecture question

- Consider an ε-NN graph, i.e. a graph with the following weights :

$$A_{ij}^{\epsilon} = \begin{cases} e^{-\frac{\text{dist}(x_i,x_j)^2}{2\epsilon^2}} & \text{if } \text{dist}(x_i,x_j) \leq \epsilon \\ 0 & \text{otherwise} \end{cases}$$

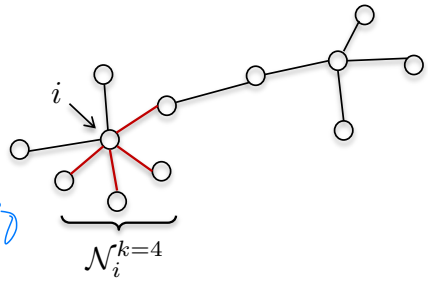
why have this here ?



ϵ-Ball

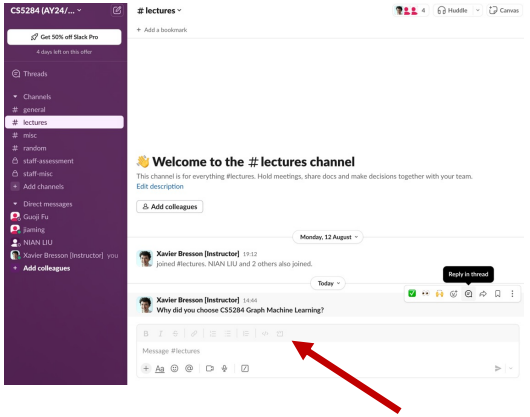
- The k-NN graph's adjacency matrix is defined as :

$$A_{ij}^{\text{kNN}} = \begin{cases} e^{-\frac{\text{dist}(x_i,x_j)^2}{\sigma^2}} & \text{if } j \in \mathcal{N}_i^k \\ 0 & \text{otherwise} \end{cases}$$



- Which graph is the most used in practice? Justify. k-NN. Lower time complexity

- In Slack #lectures
  - Identify the question and Reply in thread with a short response



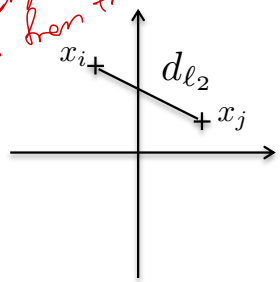
Euclidean

At high dimensions, distance between all pairs of datapoints becomes very similar → many datapoints within each ε-Ball → graph becomes very dense → less structural info → Bad

Distance definition

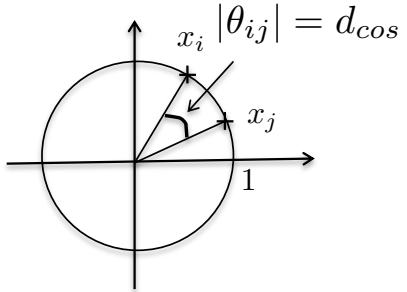
- Euclidean/L2 distance :
  - Good distance for low-dim data, e.g. d < 10.
  - Good distance for high-dim data with linearly separable data (e.g. MNIST).

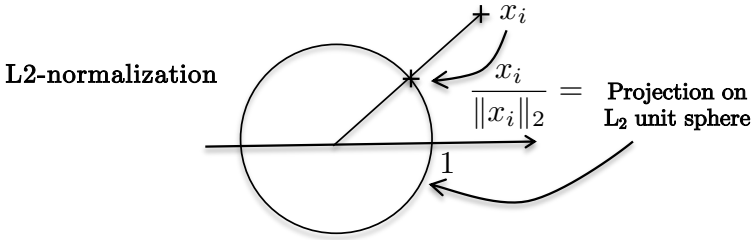
$$d_{\ell_2}(x_i, x_j) = \|x_i - x_j\|_2 = \sqrt{\sum_{m=1}^{d} |x_{i,m} - x_{j,m}|^2}$$



- Cosine/dot product distance :
  - Good distance for high-dim sparse data (e.g. text documents)

$$d_{cos}(x_i, x_j) = \left| \cos^{-1}\left(\frac{\langle x_i, x_j \rangle}{\|x_i\|_2 \|x_j\|_2} \right) \right| = |\theta_{ij}|$$





$$\underset{n \times d}{X} = \begin{bmatrix} x_1 \\ x_i \\ x_n \end{bmatrix} \quad \|x_i\|_2 = 1$$

- Other analytical distances : Kullback-Leibler distance (information theory), Wasserstein distance (optimal transport), etc.

Data features

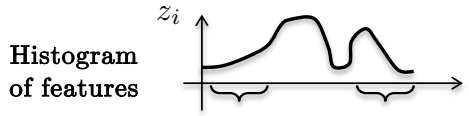
- Types of data features
  - Raw features (e.g. movie features such as genre, actors, year, etc)
  - Hand-crafted features (e.g. SIFT in computer vision, etc)
  - Learned features (PCA, NMF, sparse coding, deep learning, etc)
- It is generally unsuccessful to directly use the raw features for graph construction.
  - Issues are noise, unbalanced scaling, lack of expressiveness, curse of dimentionality, etc
- For successful graph construction, raw data should be transformed into meaningful data representation by designing new features, s.a. handcrafted or learned features.

should transform the raw data first

$$x_i \in \mathbb{R}^d \xrightarrow{\text{Feature Extraction}} z_i \in \mathbb{R}^e$$

Raw data
Ex: Image pixels

New features
Ex: Car features
Flower features



$$A_{ij} = e^{-\frac{\text{dist}(x_i, x_j)^2}{\sigma^2}}$$

$$\Downarrow$$

transformed feature

$$A_{ij} = e^{-\frac{\text{dist}(z_i, z_j)^2}{\sigma^2}}$$

Standard pre-processing

- Center data (along feature dimension) : zero-mean property

$$x_i \leftarrow x_i - \text{mean}(\{x_i\}) \in \mathbb{R}^d$$

- Normalize data variance (along feature dimension) : z-scoring property

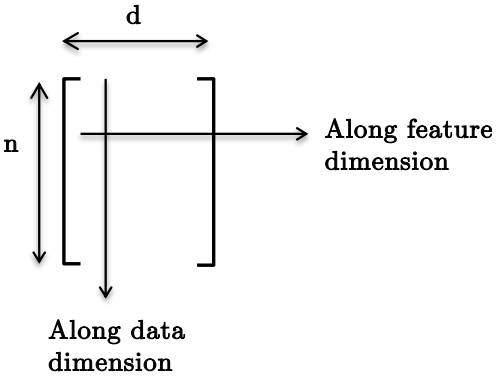
$$x_i \leftarrow x_i \ / \ \text{std}(\{x_i\}) \in \mathbb{R}^d$$

$$\text{with } \text{std}(\{x_i\})^2 = \text{mean}(\{\left(x_j - \text{mean}(\{x_i\})\right)^2\})$$

- Project data on L2-sphere (along feature dimension or data dimension) :

$$x_i \leftarrow x_i \ / \ \|x_i\|_2 \in \mathbb{R}^d$$

X =



- Normalize max and min of feature value :

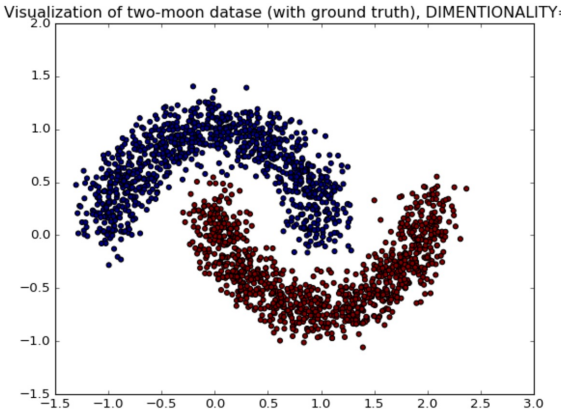
$$x_i \leftarrow \frac{x_i - \min(\{x_i\})}{\max(\{x_i\}) - \min(\{x_i\})} \in [0,1]^d$$

Lab 3 : Graph construction for two-moon

- Run code03.ipynb and study data pre-processing, construction of k-NN graphs, visualization of distances, adjacency matrix, and graph quality with clustering accuracy.

```
# Visualize in 2D
plt.figure(30)
size_vertex_plot = 20.
plt.scatter(X[:,0], X[:,1], s=size_vertex_plot*np.ones(n), c=C)
plt.title('Visualization of two-moon datase (with ground truth), DIMENTIONALITY= ' + str(dim))
plt.show()
```

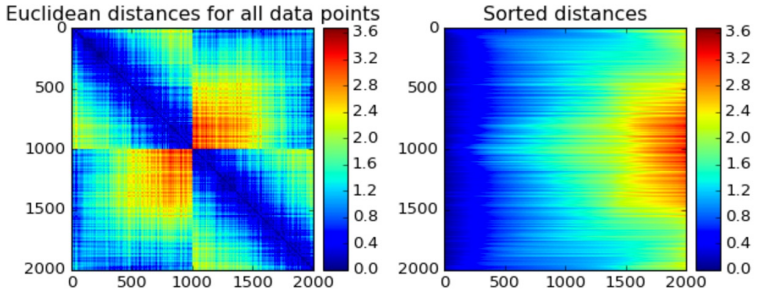
```
(2000, 2) (2000,)
```



not linearly separable data

```
In [9]: # Visualize distances
        fig, (ax1, ax2) = plt.subplots(1,2)
        #fig.suptitle('Title of figure 2', fontsize=15)

        ax1.set_title('Euclidean distances for all data points')
        im1 = ax1.imshow(Dnot_sorted, interpolation='nearest')
        divider1 = make_axes_locatable(ax1)
        cax1 = divider1.append_axes("right", size="10%", pad=0.1)
        ax1.get_figure().colorbar(im1, cax=cax1)
```

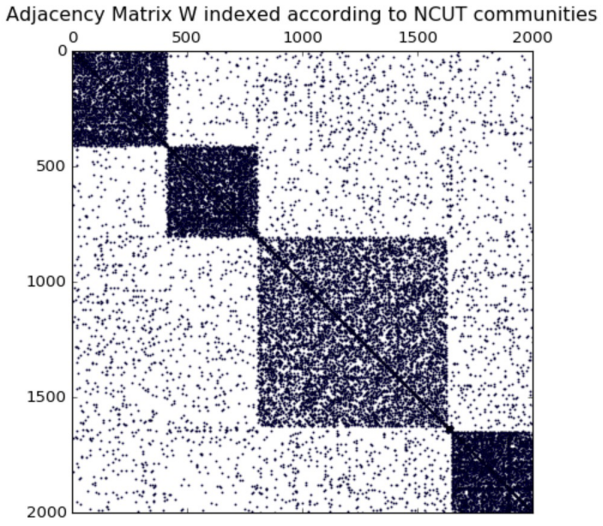


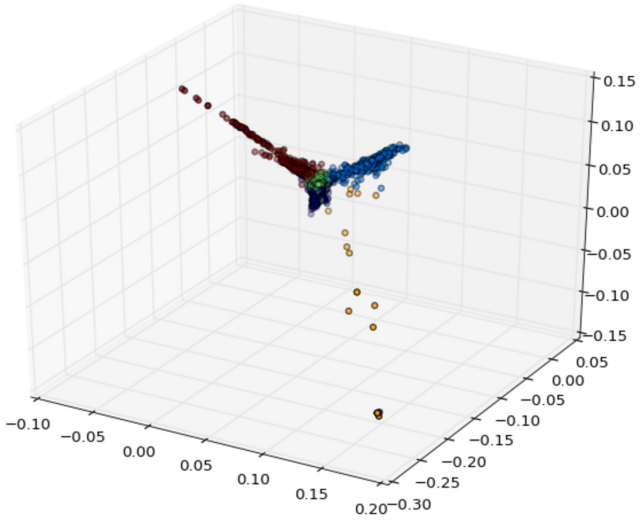
Lab 4 : Graph construction for text documents

- **Run code04.ipynb and construct graph text documents.**

```
In [9]: # Compute the k-NN graph with Cosine distance
        W_cosine = construct_knn_graph(X,10,'cosine')

        k-NN graph with cosine distance
```





Outline

- Graph theory
- Graph categories
- Basic definitions
- Curse of dimensionality and structure
- Manifolds and graphs
- Spectral graph theory
- Graph construction
- **Conclusion**

Summary

- Graphs can represent complex and heterogenous relationships between data.
  - They help to go beyond the standard assumption that data are i.i.d. (independent and identically distributed) as they explicitly leverage the connections between pairs of data.
  - Any dataset and task that use explicit relations between data is a graph-based task.
    - When we begin looking for graphs, we discover they are ubiquitous! ☺
- Graphs offer an augmented representation of data.
  - With data feature X and data relationship depicted by G = (V,E,A).

Summary

- First fundamental tool of graph science :
  - Adjacency matrix A
    - It reveals global structures in data relationship (graph spectrum).
    - It can visualize graphs in 2D or 3D Euclidean spaces (later discussed).
    - It can boost performance of machine learning techniques (later discussed).
- Second fundamental tool of graph science :
  - Graph Laplacian matrix L
    - It is a diffusion operator -- It propagates information on graphs (parabolic PDEs).
    - It is used to reveal modes of variation of the graph system.
    - It is used for image compression (jpeg), neuroscience (brain activity), positional encoding (later discussed), etc.

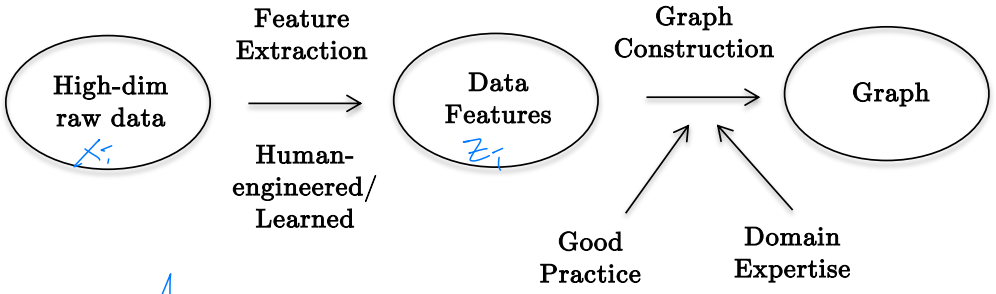
and also controls the speed of propagation

Pipeline

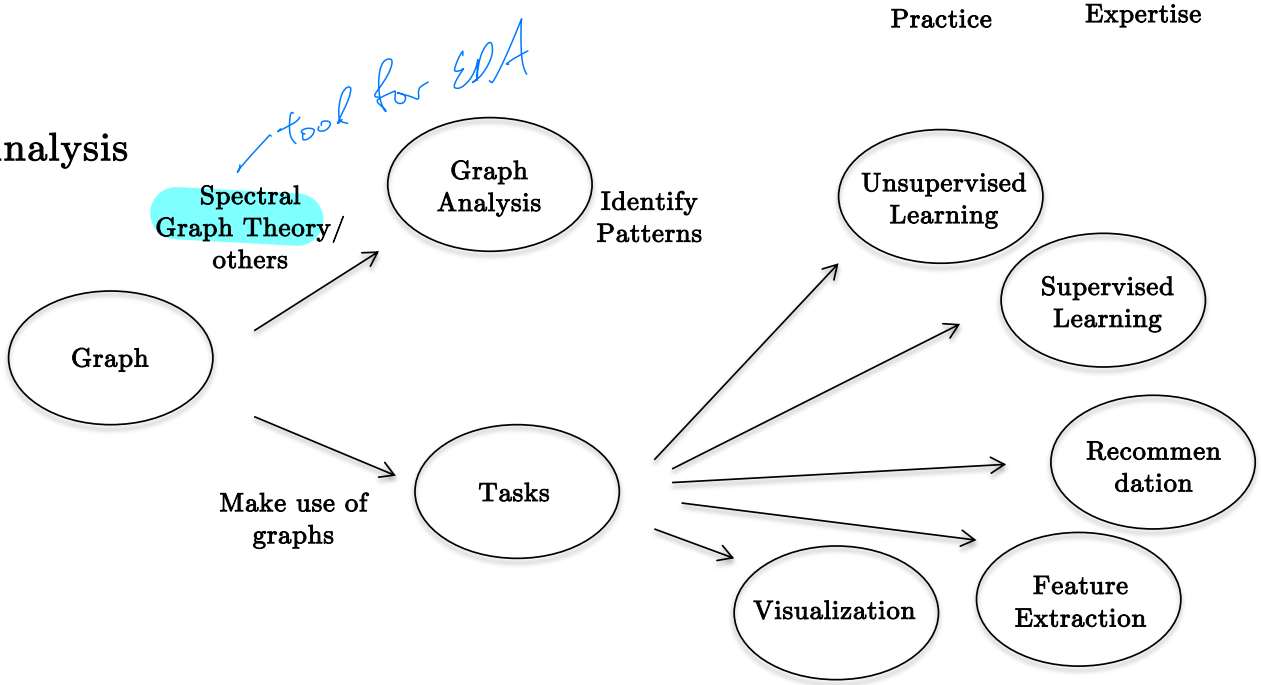
- Step #1: Data ⇒ Graph

  Skip this step if graph is given,

  e.g. molecule, social network, etc



- Step #2: Graph ⇒ Analysis



Questions?