MAT 280: Harmonic Analysis on Graphs & Networks
Lecture 9: Graph Construction from Given Datasets

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Outline

1. Motivation: How to Construct a Graph from a Given Dataset
2. Simple Graph Construction Strategies
3. Optimization Strategy by Daitch-Kelner-Spielman

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From Datasets to Graphs

- Suppose we have deployed a set of sensors at scattered (i.e., unequally-spaced) locations and each sensor records time series (or waveform) data measuring certain properties of interest, e.g.,
  - seismometers to monitor volcanic activities;
  - acoustic sensors to detect underground tunnels;
  - biosensors to detect pathogens, . . .
- In order to analyze such data in an efficient manner not only along the time axis but also *across* the sensors (i.e., the spatial directions), we need to construct a *graph* whose vertices represent the spatial locations where the sensors are placed.
- Then an important question is how to define *edges* among these vertices to form a graph.

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Unless the restrictive and predefined cases (e.g., each sensor/vertex is physically forced to connect to only a handful of its neighbors), we need to answer the following questions:

- Should we connect each vertex to every other vertex to make a *complete* graph?
- Or should we create a *sparse* graph for efficiency without deteriorating the performance of the task at hand (e.g., detection, classification, regression, missing data recovery, etc.)?
- What *weight* should we assign to each edge?

These questions are also important in completely different and more general scenarios where each vertex represents not the sensor location but simply a *vector* in $\mathbb{R}^d$ (e.g., an image patch for denoising and feature extraction, etc.)

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Criteria for Good Graphs

- What is a *good* graph?
- Obviously, this question depends on the task at hand (e.g., classification, regression, missing data recovery, . . .).
- Yet, the "goodness" of a graph should be measured in the following three criteria:

C1 Computational efficiency for constructing a graph from given data;

C2 Computational efficiency for processing data on the constructed graph;

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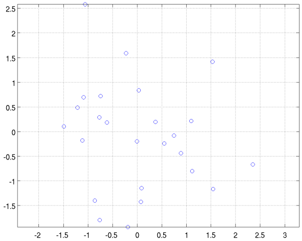
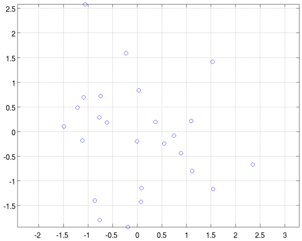


(a) Sensor locations

Three Possibilities



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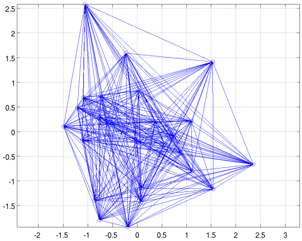

(b) Complete graph

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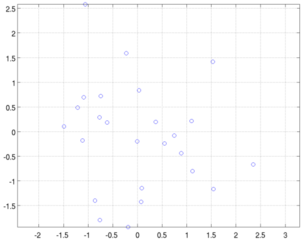

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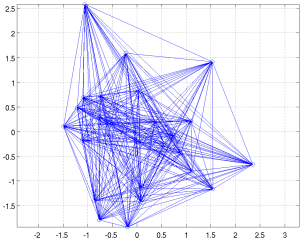

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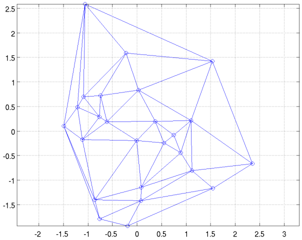

(c) Delaunay graph

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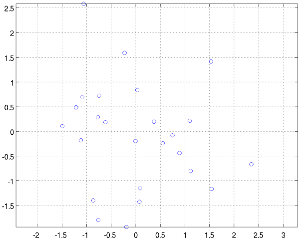

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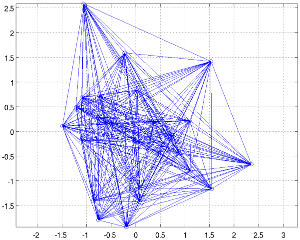

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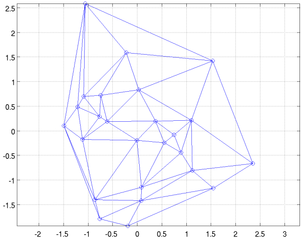

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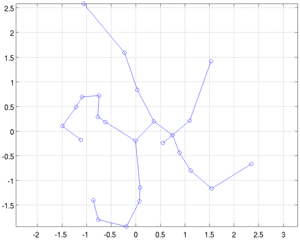

(d) Minimum spanning tree

Complete Graphs

- Construct a *complete* graph $K(V) = K_n$ by mutually connecting all the vertices $v_1, \ldots, v_n$.
- Often the Gaussian weights are used for the edge weights, i.e., for $w_{ij} = \exp(-\mathrm{dist}(v_i, v_j)^2/\epsilon^2)$ where $\mathrm{dist}(\cdot,\cdot)$ is an appropriate distance function (e.g., ℓ^2-distance), and ϵ is an appropriate scale parameter, which is often difficult to choose (more about it in the next lecture).
- This is easy and good in the sense of Criterion 1.
- Hence, many people in fact have been constructing and using this strategy more or less mindlessly.
- The number of its edges, however, is of course quite large, i.e., $|E(K_n)| = n(n-1)/2$, which may hinder it from being good in Criterion 2.

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Delaunay Graphs

- How to *sparsify* a complete graph to improve Criterion 2 while keeping Criterion 1 in mind?
- One of the possibilities may be the so-called *Delaunay graph*.
- If $v_i \in \mathbb{R}^2$, $i = 1, \dots, n$, then the *Delaunay triangulation* $DT(V)$ for V is a triangulation such that no vertex in V is inside the circumcircle of any triangle in $DT(V)$.

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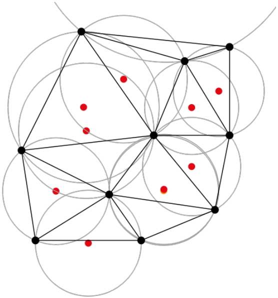

Figure: From Wikipedia

Delaunay Graphs . . .

- $DT(V)$ maximizes the minimum angle of all the angles of the triangles in the triangulations $\Longrightarrow$ tends to avoid extremely skinny triangles
- Moreover, in $\mathbb{R}^2$, there is a fast algorithm to construct $DT(V)$ with $O(n \log n)$ cost.
- A graph representing such Delaunay triangulation of V is called the *Delaunay graph* of V, and denoted by $DG(V)$.
- By considering circumscribed spheres, the notion of Delaunay triangulation can extend to three and higher dimensions.
- The computational cost to construct $DG(V)$ for higher dimension, however, can be high: $O(n \log n + n^{\lceil d/2 \rceil})$ if $V \subset \mathbb{R}^d$.
- Hence, the Delaunay graph may be useful if the vertices represent the physical sensor locations/coordinates in $\mathbb{R}^2$ or at most $\mathbb{R}^3$.
- In more general situations where each vertex directly represent a high dimensional vector in $\mathbb{R}^d$ with $d > 3$, then this may not be a good approach in terms of Criterion 1.

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- Can construct the so-called *minimum spanning tree* from either a complete graph or a Delaunay graph.
- A *spanning tree* of a given connected graph $G(V, E)$ is a subgraph of G that is a tree and connects all the vertices in V together.
- In general, G can have many different spanning trees, and the *minimum spanning tree* $MST(G)$ of G is a spanning tree whose total edge weights (i.e., the sum of the edge weights in that tree) are less than or equal to those of every other spanning tree.

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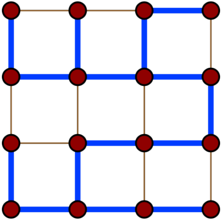
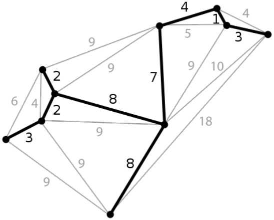


(a) MST(a lattice)



(b) MST(a weighted graph)

Figure: From Wikipedia

Minimum Spanning Trees

- It is well known that

$$MST(K(V)) \subset DG(V) \subset K(V)$$

- $MST(G)$ is the sparsest graph that connects all the vertices without redundancy; but it may not be unique for a given G.
- Computing $MST(G)$ for a given $G = G(V, E)$ is good in Criterion 1: there exists fast algorithms with the cost $O(|E(G)| \log n)$.
- This does not depends on the dimension of the vectors d at the vertices. Hence, $MST(G)$ is easier to compute than $DG(V)$ in general.
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k-Nearest Neighbor Graphs

- Yet another popular approach to construct a graph from a given dataset is the so-called *k-nearest neighbor graph*.
- Its construction is simple: connect v_i with v_j if v_j is among the k-nearest neighbors of v_i.
- This definition leads to a directed graph. To make it undirected, there are two approaches:
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The ε-Neighborhood Graph

- This graph is created by connecting all vertices whose pairwise distances are smaller than $\varepsilon > 0$.
- Since the distances between all connected vertices are roughly of the same scale (at most ε), weighting the edges would not incorporate more information about the data to the graph.
- Hence, the ε-neighborhood graph is usually viewed as an *unweighted* graph.
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Outline

1. Motivation: How to Construct a Graph from a Given Dataset
2. Simple Graph Construction Strategies
3. Optimization Strategy by Daitch-Kelner-Spielman

The Daitch-Kelner-Spielman Construction

- Given a collection of vectors $\{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n\} \subset \mathbb{R}^d$, we want to fit a good, weighted, and undirected graph to them.
- Viewing these vectors as vertices in a graph, it boils down to the following question: how to determine the weight $a_{ij} \geq 0$ between $\boldsymbol{x}_i$ and $\boldsymbol{x}_j$?
- No self-loop is allowed, i.e., $a_{ii} = 0$.
- Let $X = [\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n] \in \mathbb{R}^{d \times n}$ be the data matrix.
- DKS proposed to find the weighted adjacency matrix $A \in \mathbb{R}^{n \times n}_{\geq 0}$ and $A^{\mathsf{T}} = A$ such that

$$\min_{A \in \mathbb{R}^{n \times n}_{\geq 0};\, A^{\mathsf{T}} = A} \left\| L X^{\mathsf{T}} \right\|_F^2 = \min_{a_{ij} \geq 0} \sum_{i=1}^{n} \left\| \sum_{j=1}^{n} a_{ij} (\boldsymbol{x}_i - \boldsymbol{x}_j) \right\|_2^2 .$$

- The above objective function looks quite natural since a_{ij} becomes small if $\boldsymbol{x}_i$ and $\boldsymbol{x}_j$ are far apart.

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- To prevent this, the constraints, $d_i = \sum_{j=1}^{n} a_{ij} > 0$, $i = 1, \ldots, n$, are added in the above minimization problem.
- Furthermore, define a *hard graph* of X to be a graph minimizing $\|LX^{\mathsf{T}}\|_F^2$ subject to $d_i \geq 1$, $i = 1, \ldots, n$.
- Since some vectors could be outliers, define an *α-soft graph* of X to be a graph minimizing $\|LX^{\mathsf{T}}\|_F^2$ subject to $\sum_i (\max(0, 1 - d_i))^2 \leq \alpha n$, which constrains the number of edges with small weights.

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- Here, we will describe a couple of theorems on the properties of the hard and α-soft graphs.

Theorem (DKS, 2009)

For every $\alpha > 0$, every set of n vectors in $\mathbb{R}^d$ has a hard and an α-soft graph with at most $(d+1)n$ edges. Consequently, the average degree of a vertex in such graphs is at most $2(d+1)$.

$\Longrightarrow$ Once such a graph is constructed, the average degree of that graph can be used for the measure of the *essential dimensionality* of the input data vectors, which could be much lower than the ambient dimension d.

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Some Results from the DKS paper

- As examples, DKS used the well-known datasets from the UCI Machine Learning Repository (Asuncion & Newman, 2007) or LIBSVM (Chang & Lin, 2001).
- Performed classification, regression, and clustering experiments on these datasets.
- Here, we show only their classification results.
- Let $X = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n\}$ be the available vectors for a given classification problem, and let $T = \{\boldsymbol{x}_i\}_{i \in I_T}$ be a set of m labeled training vectors ($m < n$), and $I_T \subset N := \{1, \ldots, n\}$ is the index set for the training vectors, and $|I_T| = m$. For the 10-fold cross validation, $m \approx n/10$.
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    1. Construct a graph G from X via the DKS algorithm
    2. Let $\{c_i \in \{0,1\}\}_{i \in I_T}$ be the training dataset labels (either 0 or 1). Then, solve
    $$\widehat{\boldsymbol{y}} = \operatorname*{arg\,min}_{\boldsymbol{y} \in \mathbb{R}^n} \boldsymbol{y}^{\mathsf{T}} L(G) \boldsymbol{y} \quad \text{subject to } y_i = c_i \text{ if } i \in I_T.$$
    3. For each test vector $\boldsymbol{x}_j$, $j \in N \setminus I_T$, classify it according to the following rule:
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Classification Results from the DKS paper

Table 2. Classification error (%), 10-fold cross validation. The best result for each data set is bold. The experiments that do not perform better than ours have a grey background.

DATA SET	HARD	0.1-SOFT	KNN	THRESH	LIBSVM	FBC	AODE	HGC	NB	C4.5	BP	SMO
GLASS	27.78	28.30	**26.92**	33.30	31.44	37.56	38.27	41.64	50.55	32.37	32.68	42.64
HEART	18.18	17.81	**16.05**	16.1	17.01	16.19	16.37	17.41	16.41	21.85	16.70	16.19
IONOSPHERE	**4.75**	5.57	18.50	6.34	6.20	9.20	8.26	6.60	17.83	10.26	12.93	12.07
IRIS	4.87	4.21	4.46	6.20	**3.87**	6.27	6.00	3.93	4.47	5.27	15.20	15.13
PIMA	26.64	26.61	24.54	26.45	23.24	25.15	23.43	24.08	24.25	25.51	22.96	**22.93**
SONAR	9.16	**8.64**	13.80	14.94	11.71	22.62	20.09	30.84	32.29	26.39	21.33	22.12
VEHICLE	23.03	22.47	27.70	29.98	**14.87**	25.77	28.35	31.90	55.32	27.72	18.89	25.92
VOWEL990	1.19	0.95	2.62	0.98	**0.64**	6.54	10.36	7.30	37.10	19.80	7.27	29.39
WINE	2.92	2.62	2.86	3.64	2.57				2.54	6.80	1.98	**1.24**

FBC: Full Bayes Classifier; AODE: Averaged One-Dependence Estimators; HGC: the Hill Climbing Bayesian network learning algorithm; NB: Naive Bayesian networks; C4.5: a decision tree algorithm; BP: Back Propagation; SMO: Sequential Minimal Optimization