Lecture 2: Geometric Graphs, Predictive Graphs and Spectral Analysis

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Data Graphs

Today we discuss construction of dynamical data graphs and spectral analysis. The overarching problem is the following:

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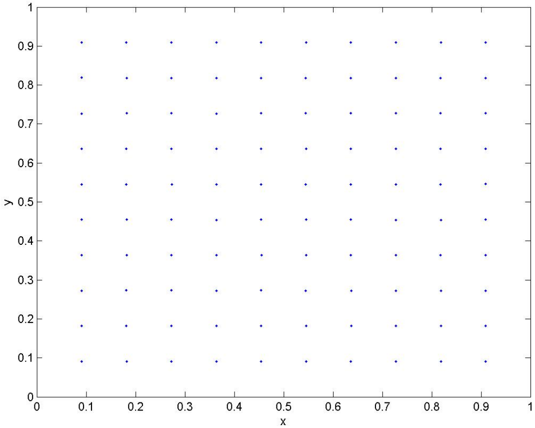
We shall discuss first how to construct a sequence of nested graphs from a data set.

Two types of data:

1. Percolation models/Geometric graphs
2. Weighted graphs

Percolation Models. Geometric graphs

Fix a set of points in $\mathbb{R}^d$. Example, for $d = 2$:



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Uniform (regular) lattice.

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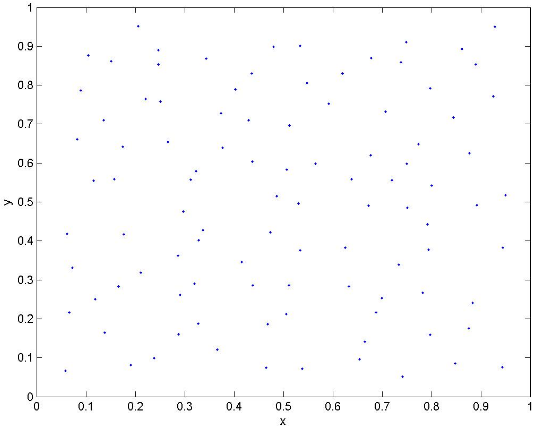

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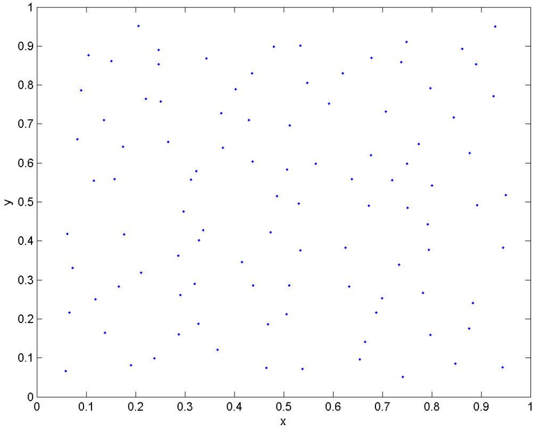

$n = 10^2 = 100$
Nonuniform (irregular) lattice.
Created by random perturbation of the regular lattice.

Percolation Models. Geometric graphs

Construct the matrix of pairwise distances:

$$V = \left(\| r^k - r^j \| \right)_{1 \leq k,j \leq n} \quad , \quad r^k = (x_k, y_k).$$

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Then sort the set of distances in an ascending order. This way we define an order on the set of pairs of points. Implicitly this defines an ascending order on the set of edges. We obtain a sequence of nested graphs

$$(G_t)_{t \geq 0} \quad 0 \leq t \leq m = n(n-1)/2$$

where t indicates the number of edges in the graph G_t.
Thus G_t has n nodes and t edges.

Percolation Models. Geometric graphs

Play Examples: $n = 100$, regular/irregular, different types of norms:

$$\|r^k - r^j\|_2 = \sqrt{(x_k - x_j)^2 + (y_k - y_j)^2}$$

$$\|r^k - r^j\|_\infty = max(|x_k - x_j|, |y_k - y_j|)$$

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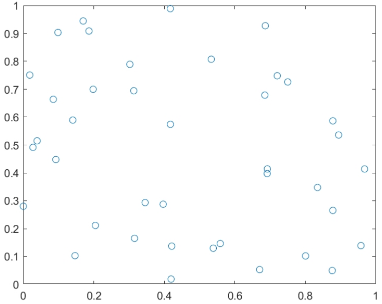

On the Bernard& Killworth office data from: http://vlado.fmf.uni-lj.si/pub/networks/data/ucinet/ucidata
Generate random 40 points in the unit square.

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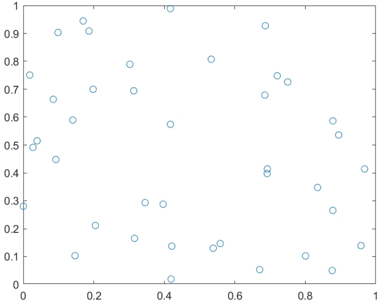

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See movie: bkoff_movie.mp4

Data Graphs
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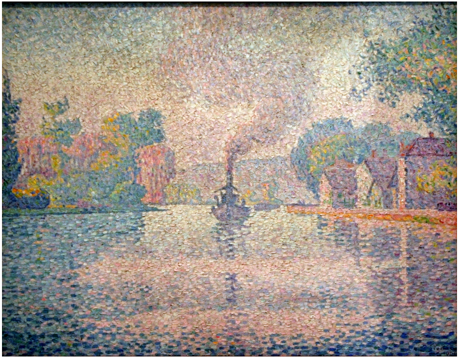

Data Graphs
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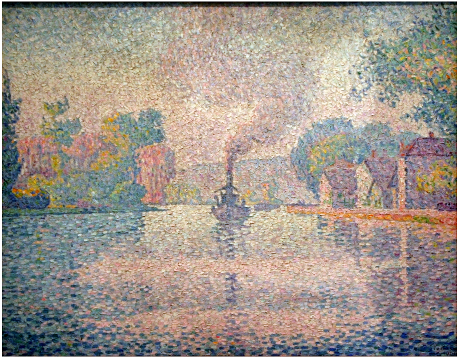

By Paul Signac - Ophelia2, Public Domain,
https://commons.wikimedia.org/w/index.php?curid=12570159
(L'Hirondelle Steamer on the Seine)

Data Graphs

Public Datasets

On Canvas you can find links to several public databases:

1. Duke: https://dnac.ssri.duke.edu/datasets.php
2. Stanford: https://snap.stanford.edu/data/
3. Uni. Koblenz: http://konect.uni-koblenz.de/
4. M. Newman (U. Michigan):
   http://www-personal.umich.edu/ mejn/netdata/
5. A.L. Barabasi (U. Notre Dame):
   http://www3.nd.edu/ networks/resources.htm
6. UCI: https://networkdata.ics.uci.edu/resources.php
7. Google/YouTube: https://research.google.com/youtube8m/

Spectral Analysis
Basic Properties

Last time we learned how to construct: the Adjacency matrix A, the Degree matrix D, the (unnormalized symmetric) graph Laplacian matrix $\Delta = D - A$, the normalized Laplacian matrix $\tilde{\Delta} = D^{-1/2}\Delta D^{-1/2}$, and the normalized asymmetric Laplacian matrix $L = D^{-1}\Delta$.

Spectral Analysis

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We denote: n the number of vertices (also known as the *size* of the graph), m the number of edges, $d(v)$ the degree of vertex v, $d(i,j)$ the distance between vertex i and vertex j (length of the shortest path connecting i to j), and by D the diameter of the graph (the largest distance between two vertices = "longest shortest path").

Spectral Analysis
Basic Properties

In this section we summarize spectral properties of the Laplacian matrices.

Theorem

1. $\Delta = \Delta^T \geq 0$, $\tilde{\Delta} = \tilde{\Delta}^T \geq 0$ *are positive semidefinite matrices.*
2. $eigs(\tilde{\Delta}) = eigs(L) \subset [0, 2]$.
3. 0 *is always an eigenvalue of* Δ, $\tilde{\Delta}$, L *with same multiplicity. Its multiplicity is equal to the number of connected components of the graph.*
4. $\lambda_{max}(\Delta) \leq 2 \max_v d(v)$, *i.e. the lagest eigenvalue of* Δ *is bounded by twice the largest degree of the graph.*

Spectral Analysis
Basic Properties

Theorem

Let $0 = \lambda_0 \leq \lambda_1 \leq \cdots \leq \lambda_{n-1} \leq 2$ *be the eigenvalues of* $\tilde{\Delta}$ *(or* L*), that is* $eigs(\tilde{\Delta}) = \{\lambda_0, \lambda_1, \cdots, \lambda_{n-1}\} = eigs(L)$*. Then:*

1. $\sum_{i=0}^{n-1} \lambda_i \leq n$.
2. $\sum_{i=0}^{n-1} \lambda_i = n - \#\text{isolated vertices}$.
3. $\lambda_1 \leq \frac{n}{n-1}$.
4. $\lambda_1 = \frac{n}{n-1}$ *if and only if the graph is complete (i.e. any two vertices are connected by an edge).*
5. *If the graph is not complete then* $\lambda_1 \leq 1$.
6. *If the graph is connected then* $\lambda_1 > 0$*. If* $\lambda_i = 0$ *and* $\lambda_{i+1} \neq 0$ *then the graph has exactly* $i+1$ *connected components.*
7. *If the graph is connected (no isolated vertices) then* $\lambda_{n-1} \geq \frac{n}{n-1}$.

Spectral Analysis

Smallest nonnegative eigenvalue

Theorem

Assume the graph is connected. Thus $\lambda_1 > 0$. *Denote by* D *its diameter and by* $d_{max}, \bar{d}, d_H$ *the maximum, average, and harmonic avergae of the degrees* $(d_1, \cdots, d_n)$*:*

$$d_{max} = \max_j d_j \quad , \quad \bar{d} = \frac{1}{n}\sum_{j=1}^{n} d_j \quad , \quad \frac{1}{d_H} = \frac{1}{n}\sum_{j=1}^{n} \frac{1}{d_j}.$$

Then

1. $\lambda_1 \geq \frac{1}{nD}$.
2. *Let* $\mu = \max_{1 \leq j \leq n-1} |1 - \lambda_j|$. *Then*

$$1 + (n-1)\mu^2 \geq \frac{n}{d_H}(1 - (1+\mu)(\frac{\bar{d}}{d_H} - 1)).$$

Spectral Analysis
Smallest nonnegative eigenvalue

Theorem

[continued]

3. *Assume $D \geq 4$. Then*

$$\lambda_1 \leq 1 - 2\frac{\sqrt{d_{max} - 1}}{d_{max}}(1 - \frac{2}{D}) + \frac{2}{D}.$$

Spectral Analysis

Comments on the proof

"Ingredients" and key relations:

1. Let $f = (f_1, f_2, \cdots, f_n) \in \mathbb{R}^n$ be a n-vector. Then:

$$\langle \Delta f, f \rangle = \sum_{x \sim y} (f_x - f_y)^2$$

where $x \sim y$ if there is an edge between vertex x and vertex y (i.e. $A_{x,y} = 1$).

This proves positivity of all operators.

2. Last time we showed $eigs(\tilde{\Delta}) = eigs(L)$ because $\tilde{\Delta}$ and L are similar matrices.

3. 0 is an eigenvalue for Δ with eigenvector $1 = (1, 1, \cdots, 1)$. If multiple connected components, define such a 1 vector for each component (and 0 on rest).

4. $\lambda_{max}(\tilde{\Delta}) = 1 - \lambda_{min}(D^{-1/2} A D^{-1/2}) \leq 1 + |\lambda_{min}(D^{-1/2} A D^{-1/2})|$.

Spectral Analysis

Comments on the proof - 2

$$\lambda_{max}(D^{-1/2}AD^{-1/2}) = \max_{\|f\|=1} \langle D^{-1/2}AD^{-1/2}f, f\rangle = \max_{\|f\|=1} \sum_{i,j} A_{i,j} \frac{f_i}{\sqrt{d_i}} \frac{f_j}{\sqrt{d_j}}$$

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Next use Cauchy-Schwartz to get

$$\left|\sum_{i,j} A_{i,j} \frac{f_i}{\sqrt{d_i}} \frac{f_j}{\sqrt{d_j}}\right| \leq \sum_i \frac{f_i^2}{d_i} \sum_j A_{i,j} = \sum_i f_i^2 = \|f\|^2 = 1.$$

Thus $\lambda_{max}(\tilde{\Delta}) \leq 2$. Similarly $\lambda_{max}(\Delta) \leq 2(\max_i d_i)$.

Spectral Analysis

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Consequence: The normalized Laplacian has the following eigenvalues:

1. For cycle graph on n vertices: $\lambda_k = 1 - cos\frac{2\pi k}{n}$, $0 \leq k \leq n-1$.
2. For the complete graph on n vertices:

$$\lambda_0 = 0\ ,\ \lambda_1 = \cdots = \lambda_{n-1} = \frac{n}{n-1}.$$

References

- B. Bollobás, **Graph Theory. An Introductory Course**, Springer-Verlag 1979. **99**(25), 15879–15882 (2002).
- F. Chung, **Spectral Graph Theory**, AMS 1997.
- F. Chung, L. Lu, The average distances in random graphs with given expected degrees, Proc. Nat.Acad.Sci. 2002.
- R. Diestel, **Graph Theory**, 3rd Edition, Springer-Verlag 2005.
- P. Erdös, A. Rényi, On The Evolution of Random Graphs
- G. Grimmett, **Probability on Graphs. Random Processes on Graphs and Lattices**, Cambridge Press 2010.
- J. Leskovec, J. Kleinberg, C. Faloutsos, Graph Evolution: Densification and Shrinking Diameters, ACM Trans. on Knowl.Disc.Data, **1**(1) 2007.