

LAPLACIAN MATRIX OF A NETWORK AND APPLICATIONS



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- 1 Over view of Networks
- 2 Laplacian Matrix
- 3 Applications of Laplacian Matrix
 - Laplacian Centrality
 - Diffusion on networks
- 4 Generalised Heat Diffusion Model
- 5 Heat Kernel of a Graph

Introduction to Networks

- Intuition of Networks

Whenever one mentions the word 'network', one normally thinks of an interconnection of items or things.

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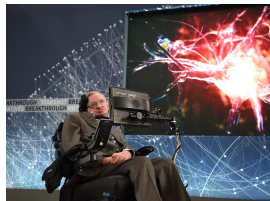
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- Did you know?

network:
all the time, everywhere with everybody

Complexity & Complex Systems

"I think the next century will be
a century of complexity" -
Stephen Hawking



Complexity and Complex Systems cont...

Complex

[adj., v. kuh m-pleks, kom-pleks; n. kom-pleks]
-adjective

1.
composed of many interconnected parts;
compound; composite: a complex highway
system.

2.
characterized by a very complicated or
involved arrangement of parts, units, etc.:
complex machinery.

3.
so complicated or intricate as to be hard to
understand or deal with: a complex problem.

Source: Dictionary.com

Complexity, a **scientific theory** which asserts that some systems display behavioral phenomena that are completely inexplicable by any conventional analysis of the systems' constituent parts. These phenomena, commonly referred to as emergent behaviour, seem to occur in many complex systems involving living organisms, such as a stock market or the human brain.

Source: John L. Casti, Encyclopædia Britannica

Complexity



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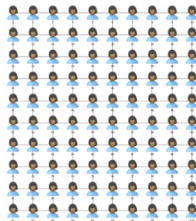


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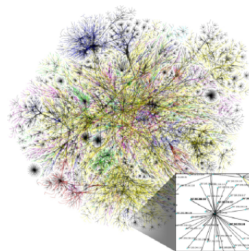


Complex Networks

- Complex Networks represent skeletons of complex systems
- Complex networks exhibit a **non-trivial topology**



(g) grid lattice



(h) internet

Network Approach to Complex System Study

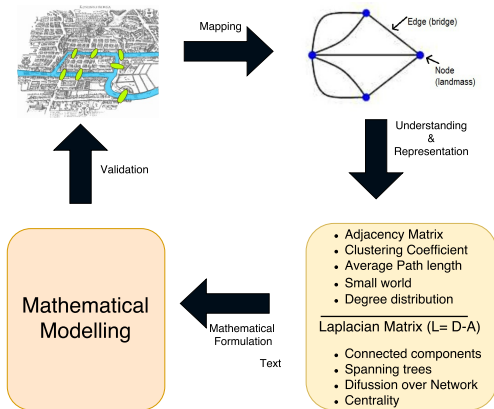
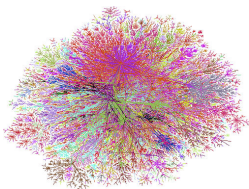


Figure: Illustration of the process of network theory approach

Real-world Networks

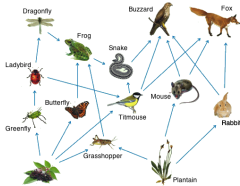


(a) Internet

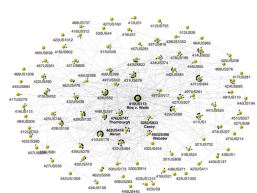


Nature Reviews | Genetics

(b) Protein-Protein



(c) Food web



(d) Citation network

Source: www.wikipedia.com

AIMS,SA 2016-2017 Friendship Network

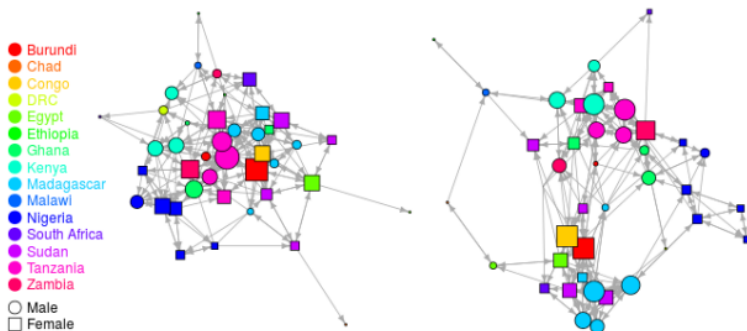


Figure: AIMS,SA 2016-2017 Friendship Network: December (left) and April (right). The size of each node is proportional to in-degree (close friends).

Source: Emily Muller, Master's Thesis

Laplacian Matrix

Definition

For a simple undirected graph;

$$L = D - A, \quad (1)$$

where D is the $\text{diag}(k_i)$ and $A_{i,j} = 1$ if $i \sim j$ and 0 otherwise.

The entries of L are given by

$$L_{i,j} = \begin{cases} k_i & \text{if } i = j \\ -1 & \text{if } i \neq j \text{ and } i \sim j \\ 0 & \text{otherwise,} \end{cases} \quad (2)$$

where k_i denotes the degree of node i (Estrada, 2011).

Spectrum of the Laplacian Matrix

Spectrum

Spectrum of a matrix is a set eigenvalues and their multiplicities. Let λ_i denote the eigenvalues of the Laplacian matrix. Considering the nondecreasing order: $\lambda_n \geq \lambda_{n-1} \geq \cdots \geq \lambda_2 \geq \lambda_1 = 0$

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Insights from spectrum

- The multiplicity of 0 as an eigenvalue of \mathbf{L} is equal to the number of connected components in the network.
- A network, G , is connected if its second smallest eigenvalue is nonzero. That is, $\lambda_2 > 0$ if and only if G is connected. The eigenvalue λ_2 is thus called the algebraic connectivity of a network, $a(G)$ (Estrada, 2011).

Applications of Laplacian Matrix

- Centrality measure
- Diffusion on network
- Consensus in multi-agent systems
- Synchronization, etc

Centrality Measures

In networks, centrality is the measure how important/central a node is, in the network (Newman, 2010). There exists various measures such as:

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- **Eigenvector** centrality: Improvement in degree centrality
- **Subgraph** centrality: Participation of a node in subgraphs in network
- **Laplacian** centrality : Impact of deactivation/removal of a node from the network.

Laplacian Centrality: motivation

- There is a growing need for centrality measures for weighted networks since these networks contain rich information (Qi et al., 2012).

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- The Laplacian centrality is a measure between local and global (i.e intermediate) characterisation of the centrality of a node.

Laplacian Centrality Cont....

Laplacian Energy of a Network

The importance of a node is determined by the ability of the network to respond to the deactivation of a node from the network.

The response is quantified by the relative drop in Laplacian energy (E_L) of the network (Qi et al., 2012).

$$E_L(G) = \sum_{i=1}^n \lambda_i^2 = \sum_{i=1}^n x_i^2 + 2 \sum_{i < j} w_{ij}^2, \quad (3)$$

where x_i 's are vertex sums and w_{ij} are weights of edges between vertices i and j (Qi et al., 2012).

Mathematical Formulation of Laplacian Centrality

Mathematically, Laplacian centrality for a node i in network G is given by (Qi et al., 2012)

$$C_L(v_i, G) = \frac{(\Delta E)_i}{E_L(G)} = \frac{E_L(G) - E_L(G_i)}{E_L(G)}, \quad (4)$$

where

$E_L(G)$ - Laplacian energy of network G .

$E_L(G_i)$ - Laplacian energy of network G on removal of node i

Graph Theoretical Interpretation of Laplacian Centrality

Expressing Equation 4 in terms of 2-walks of the node i gives

$$(\Delta E)_i = 2 \cdot NW_2^M(v_i) + 2 \cdot NW_2^E(v_i) + 4 \cdot NW_2^C(v_i), \quad (5)$$

where

- $NW_2^C(v_i)$ - closed 2-walks containing vertex v_i ,
- $NW_2^E(v_i)$ - non-closed 2-walks with v_i as one of the end points,
- $NW_2^M(v_i)$ - non-closed 2-walks with v_i as the middle point.

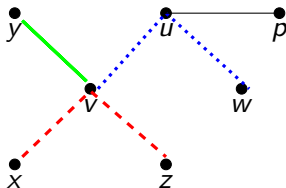


Figure: 2-walks at node v

Application to Zachary's Karate Network

- **The Zachary's Karate Network** was created from a dataset formed by observation of 34 members of a karate club over two years. Misunderstandings within the group led to a split into two groups, one led by the Administrator (1) and the other by the instructor (34).

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- **Edges** represent **interactions** outside karate activities.
- The **weights** on the edges correspond to various **activities** of interactions between players
- Database Source: http://nexus.igraph.org/api/dataset_info?id=1&format=html

Zachary's Karate Network cont...

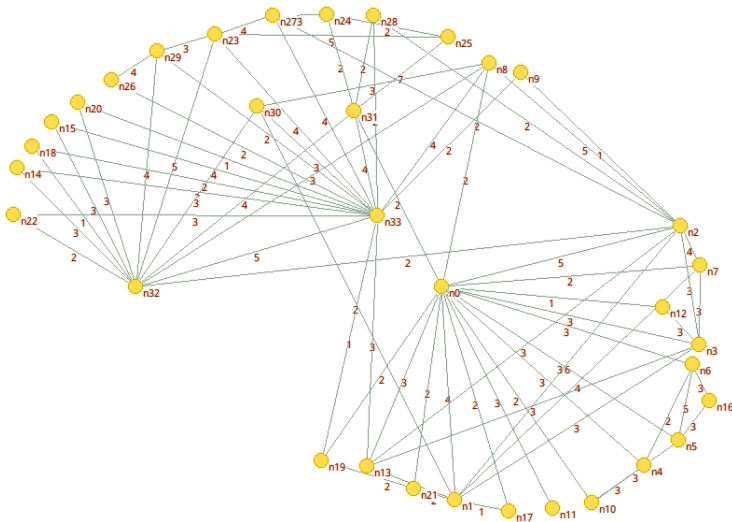


Figure: Zachary's Karate Network

Interpretations of Results

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- For all the other centralities mentioned earlier and the Laplacian centrality, both the administrator and Instructor scored highly.
- There is a good positive correlation between the degree and the Laplacian centralities.

Diffusion on networks

Diffusion is a process by which information, epidemic, viruses, and any other behaviours spread over networks [?]. Take a simple undirected connected network. Consider a quantity of substance ϕ_i (heat) at each node i at time t . The diffusion of heat over the network is given by

$$\frac{d\phi}{dt} + C\mathbf{L}\phi = 0, \quad \phi(0) = \phi_0 \quad (6)$$

Equilibrium behaviour

As time t goes to infinity, the equilibrium state is completely determined by the **kernel of \mathbf{L}** . The quantity of heat $\phi_j(t)$ at any node j at time t is given by

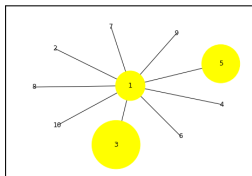
$$\lim_{t \rightarrow \infty} \phi_j(t) = \frac{1}{n} \sum_{i=1}^n \phi_i(0).$$

NOTE:

The structure of the network has no influence over the equilibrium value but plays a role in influencing the rate at which diffusion occurs.

Illustration of diffusion over a simple network

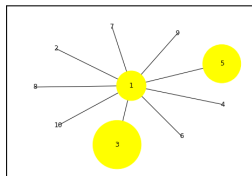
Suppose we assign to each node heat quantities given by $\phi_0 = [2, 0, 8, 0, 5, 0, 0, 0, 0, 0]$ in order node 1 to 10. Let $C = 1$.



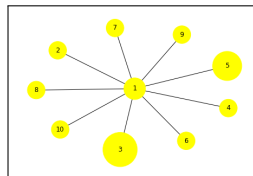
(a) $t = 0$

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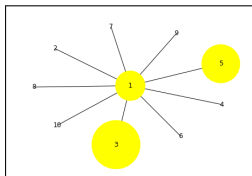
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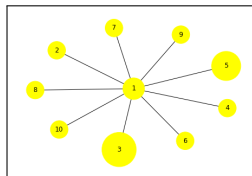
(b) $t = 1$

Illustration of diffusion over a simple network

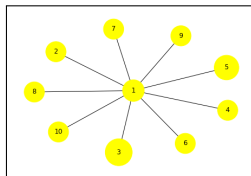
Suppose we assign to each node heat quantities given by $\phi_0 = [2, 0, 8, 0, 5, 0, 0, 0, 0, 0]$ in order node 1 to 10. Let $C = 1$.



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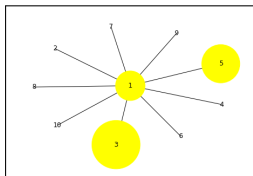
(b) $t = 1$



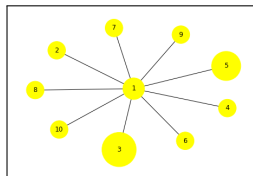
(c) $t = 2$

Illustration of diffusion over a simple network

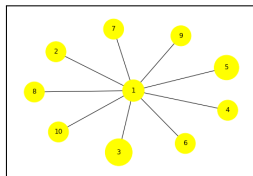
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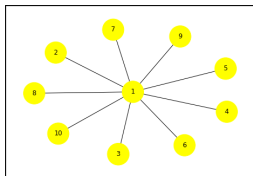
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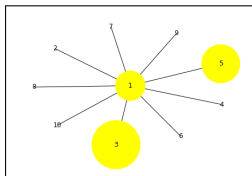
(c) $t = 2$



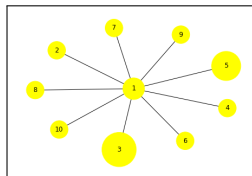
(d) $t = 5$

Illustration of diffusion over a simple network

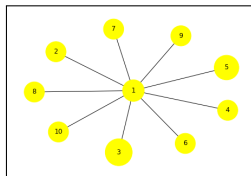
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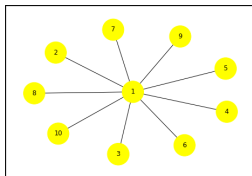
(a) $t = 0$



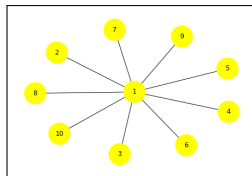
(b) $t = 1$



(c) $t = 2$



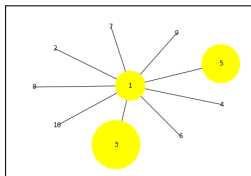
(d) $t = 5$



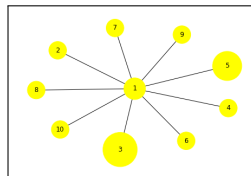
(e) $t = 7$

Illustration of diffusion over a simple network

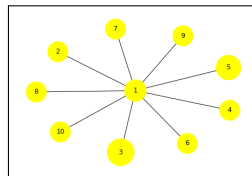
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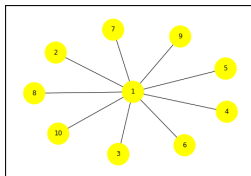
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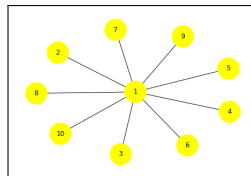
(b) $t = 1$



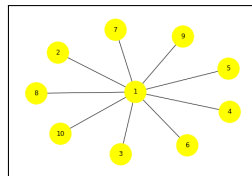
(c) $t = 2$



(d) $t = 5$

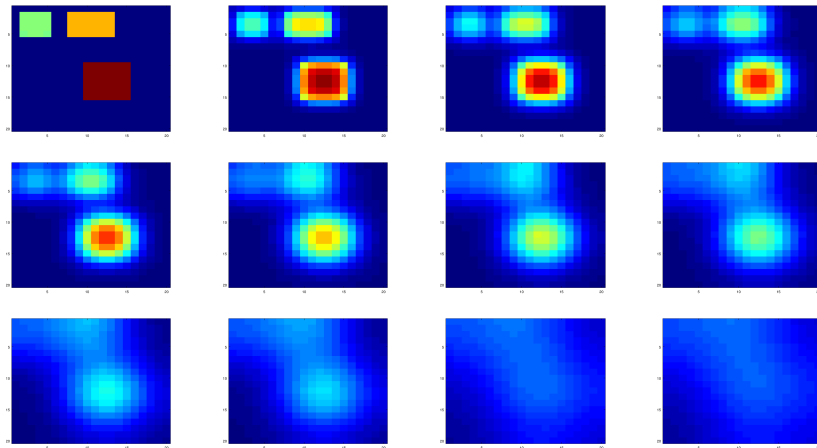


(e) $t = 7$



(f) $t = 9$

Diffusion on a Lattice



Animation: www.wikipedia.com/laplacian_matrix

Generalised Heat Diffusion Model

- Polarisation Analogy on Networks

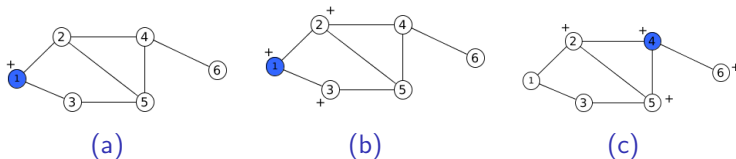


Figure: Illustration of how the polarisation analogy used as a motivation for the k -path Laplacian concept for networks.

Generalised Heat Diffusion Model Cont...

- k -path Laplacian Matrices are given by (Estrada et al., 2012)

$$L_k(ij) = \begin{cases} -1 & \text{if } d_{i,j} = k, \\ \delta_k(i) & \text{if } i = j, \\ 0 & \text{otherwise,} \end{cases} \quad (7)$$

where

$d_{i,j}$ is the shortest path distance between nodes i and j ,
 $\delta_k(i)$ known as the k -path degree.

k -path Laplacian Example

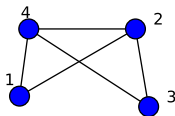


Figure: A network of size 4.

$$\mathbf{L}_1(\mathbf{G}) = \begin{pmatrix} 2 & -1 & 0 & -1 \\ -1 & 3 & -1 & -1 \\ 0 & -1 & 2 & -1 \\ -1 & -1 & -1 & 3 \end{pmatrix}, \quad \mathbf{L}_2(\mathbf{G}) = \begin{pmatrix} 1 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

Generalised Laplacian Matrix

- The generalised Laplacian matrix, L_G , is given by

$$L_G = \sum_{k=1}^{\Delta} c_k L_k \quad (8)$$

where $1 \leq \Delta \leq d_{max}$ and c_k are the coefficients.

- The values of c_k are expected to give more weight to shorter than to the longer range interactions. Some commonly used co-efficients are k^{-s} , $e^{-\lambda k}$, etc.

Generalised Diffusion Model...cont...

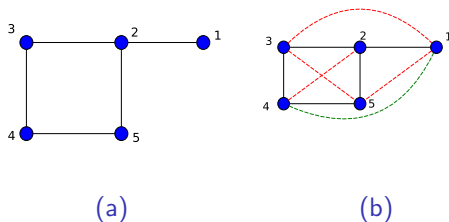


Figure: (a) is a simple graph. (b) illustrates the long-range interaction on the graph.

- The diffusion with longrange interactions is described by

$$\frac{d\phi}{dt} = -C\mathbf{L}_G\phi, \quad \phi(0) = \phi_0 \quad (9)$$

Heat Kernel, H_t

- The heat kernel is the fundamental solution of equation of the diffusion equation (6).

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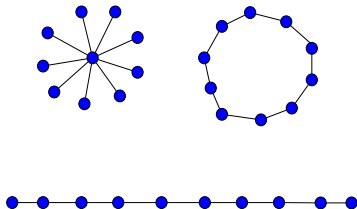
- It literally describes the flow of substance (heat) across edges (direct interactions) in the graph.

Trace of the Heat kernel

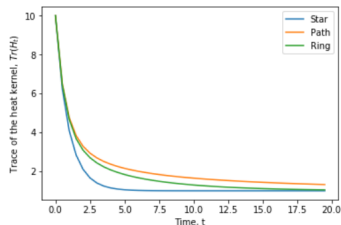
The trace of the heat kernel $Tr(H_t)$ is given by

$$Z(t) = Tr(H_t) = Tr(e^{(-\Lambda t)}) = \sum_{i=1}^{|V|} e^{-\lambda_i t}, \quad (11)$$

where λ_i is the eigenvalue of the normalised Laplacian matrix.



(a)



(b)

Zeta Function

- The Zeta function associated with the Laplacian eigenvalues is obtained by exponentiating and summing the reciprocal of the non-zero Laplacian eigenvalues.

Zeta Function

- The Zeta function associated with the Laplacian eigenvalues is obtained by exponentiating and summing the reciprocal of the non-zero Laplacian eigenvalues.
- It is thus defined by [5]

$$\zeta(s) = \sum_{\lambda_i \neq 0} \lambda_i^{-s}. \quad (12)$$

Application of Heat Kernel Invariants in Image Clustering

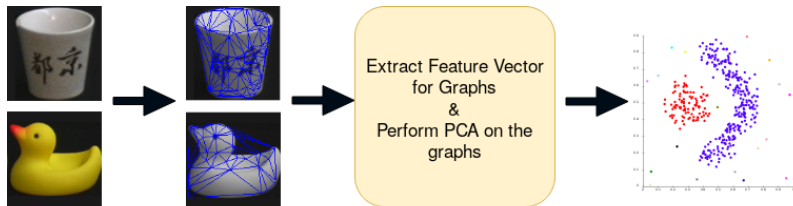


Figure: Illustration of Image Clustering process]

Summary

- Introduction to Networks and network theory approach to Complex systems study.
- Laplacian matrix and its application namely Centrality measure and Diffusion.
- Heat kernel and its use in graph characterisation
- Image clustering using heat kernel invariants
- Further work: Considering other heat kernel invariants with aim of obtaining better image clustering.

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