# Long range interactions

Alice NANYANZI (alicenanyanzi@aims.ac.za)

October 15, 2017

# Content

# 1 Diffusion of heat

## 1.1 Diffusion kernel (construct lemma and it's proof)

## 1.2 Long-range interactions based on social distance in diffusion

## 1.3 k-path Laplacians (consider Mellin and Laplace transforms to account for long-range interactions in diffusion).

# 2 Real-world Applications

## 2.1 Image Segmentation with k-path Laplacians

## 2.2 Consensus with k-path Laplacians

## 2.3 Financial risk and contagion (too interconnected to fail and centralities)

## 2.4 Frequency overlap - Design of transmitters

## 2.5 Sensor monitoring as an application of diffusion

# 3 Future Considerations

## 3.1 Centrality measures such as leverage and super diffusion centralities

## 3.2 neural correlates to future value of information (something in line is about reinforcement learning)

## 3.3 Communicability in networks

# Overview of Networks

In the study of networks or graphs, we use various terminology. Let us explore some of these terminology that we will encounter in this work.

**shortest path**

**Diameter**

# Diffusion in Networks

Diffusion is, among others, the movement of substance from a region of high concentration to a region of low concentration. Such substances include heat, gas, etc. We can consider the diffusion process over a network to build simple models of spread of a disease, information, etc. across a network [25].

Consider a simple undirected network on $n$ vertices. Let $\phi_i$ be the quantity of substance (in this case heat) on each vertex $i$ at time $t$. Since we are accounting for only direct interactions, we assume the substance spreads along edges from node $j$ to an adjacent node $i$ at a rate $C(\phi_j - \phi_i)$, where $C$ is the diffusion constant ($C > 0$). The amount of substance moving from $j$ to $i$ in a small time interval $dt$ is $C(\phi_j - \phi_i)\, dt$. Then the rate at which substance $\phi_i$ changes is given by

$$\frac{d\phi_i}{dt} = C \sum_j A_{ij}(\phi_j - \phi_i) = C \sum_j A_{ij}\phi_j - C\phi_i \sum_j A_{ij} = C \sum_j A_{ij}\phi_j - C\phi_i k_i.$$

Thus,

$$\frac{d\phi_i}{dt} = C \sum_j (A_{ij} - \delta_{ij}k_i)\phi_j, \tag{1}$$

where $\mathbf{A}$ is the adjacency matrix, $k_i$ is the degree of node $i$, and $\delta_{ij}$ is the Kronecker delta whose value is 1 if $i = j$ and 0 otherwise. In matrix-vector notation, we have

$$\frac{d\boldsymbol{\phi}}{dt} + C\mathbf{L}\boldsymbol{\phi} = 0, \quad \boldsymbol{\phi}(0) = \boldsymbol{\phi}_0. \tag{2}$$

We observe that Equation (2) is similar to that of the ordinary heat equation $\left(\frac{du}{dt} - \alpha \nabla^2 u = 0\right)$ where the Laplace operator $\nabla^2$ is replaced by the Laplacian matrix $\mathbf{L}$. Thus, the Laplacian matrix is called the Graph Laplacian. The matrix solution to Equation (2) is given as

$$\boldsymbol{\phi}(t) = \boldsymbol{\phi}_0\, e^{-C\mathbf{L}t}. \tag{3}$$

The solution vector $\boldsymbol{\phi}(t)$ can also be found as a linear combination of eigenvector $\mathbf{v}_i$ of the Laplacian matrix $\mathbf{L}$ That is,

$$\boldsymbol{\phi}(t) = \sum_i a_i(t)\mathbf{v}_i. \tag{4}$$

Introducing Equation (4) in the left hand side of Equation (2) and after algebraic manipulation we get

$$\frac{da_i}{dt} + C\lambda_i a_i = 0, i = 1, \cdots, n, \tag{5}$$

whose solution is

$$a_i(t) = a_i(0)e^{-C\lambda_i t}. \tag{6}$$

Thus,

$$\boldsymbol{\phi}(t) = \sum_i a_i(0)e^{-C\lambda_i t}\mathbf{v}_i,$$

where $a_i(0), \lambda_i$, and $\mathbf{v}_i$ are the initial condition, eigenvalues and eigenvectors of the Laplacian matrix respectively. As the Laplacian matrix is symmetric, its set of eigenvectors is orthonormal and $a_i(0)$ in terms of $\boldsymbol{\phi}(0)$ can be found simply by projection of $\boldsymbol{\phi}(0)$ onto the set of eigenvectors, i.e.

$$a_i(0) = \langle \boldsymbol{\phi}(0), \mathbf{v}_i \rangle \quad i = 1, \cdots, n. \tag{7}$$

As discussed earlier, the eigenvalues $\lambda_i$ of $\mathbf{L}$ are non-negative which implies that the solution to the diffusion equation either decays exponentially or remains constant which implies that equilibrium can be attained. Thus, given $\lambda_i$ and the initial condition $a_i(0)$, we can find the solution at any time $t$.

## 3.4 Equilibrium Behaviour

As $t$ goes to infinity, we have

$$\lim_{t \to \infty} e^{-C\lambda_i t} = \begin{cases} 0 & \text{if } \lambda_i > 0 \\ 1 & \text{if } \lambda_i = 0, \end{cases} \tag{8}$$

Asymptotically, the equilibrium state is completely determined by the kernel of $\mathbf{L}$. Since $\sum_j \mathbf{L}_{ij} = 0$, it is easy to see that $\mathbf{v^1} = \frac{1}{\sqrt{n}}[1, \cdots, 1]$, the eigenvector associated with $\lambda_i = 0$, is in the kernel of $\mathbf{L}$. We then have

$$\lim_{t \to \infty} \boldsymbol{\phi}(t) = \langle \boldsymbol{\phi}(0), \mathbf{v^1} \rangle \mathbf{v^1}. \tag{9}$$

The quantity of heat $\phi_j(t)$ at any node $j$ at time $t$ is given by

$$\lim_{t \to \infty} \phi_j(t) = \frac{1}{n} \sum_{i=1}^{n} \phi_i(0). \tag{10}$$

At equilibrium, the value of $\phi_j(t)$ converges to the same value at each of the nodes in the network, which is the average of the initial values at all nodes. This is because, as expected, neighboring nodes in the network will exchange heat until heat is spread out evenly throughout all nodes that are connected to each other.

In order to interpret and understand the heat diffusion process explained above, let us consider a small graph of size 10 as shown in Fig. 1(a). Suppose the quantity of heat at each node at time $t = 0$ is given by the vector $\boldsymbol{\phi}(0) = [3, 0, 8, 0, 5, 2, 0, 0, 0, 2]$ in the order node 1 to node 10. Let $C = 1$. We observe that at each time step $t$, nodes that initially have high amounts of heat (i.e $1, 3, 5, 6$, and $10$) exchange heat with adjacent nodes that initially had small or no heat (cool nodes). The latter gain heat from the neighbors with relatively high heat content and eventually all nodes in the network have relatively equal amounts of heat as illustrated in Fig. 1(b). At this point, all nodes are approaching the equilibrium point. At $t = 9$, the quantity of heat at each node is $\boldsymbol{\phi}(9) = [0.20038, 0.20038, 0.20031, 0.20054, 0.19987, 0.20067, 0.19972, 0.19962, 0.19934, 0.19918]$. This explains the fact that as time $t$ increases, the quantity of heat $\boldsymbol{\phi}_j(t)$ at each node tends to the equilibrium value (which is the average of the initial quantities at all nodes) of 1.6.

Let us consider two other networks of different structures that is a star network and a regular network. We explore how diffusion occurs on networks of different structures and what impact the structure of the network has on the diffusion of a network.

To begin with, taking a star network in Fig. 2(a). Suppose the initial quantity of heat at the nodes is $\boldsymbol{\phi}(0) = [3, 0, 8, 0, 5, 2, 0, 0, 0, 2]$ and let $C = 1$. The spread of heat over the network is illustrated in Fig. 2(b).We observe that the quantity of heat at node 1 (central node)drops so fast. This is because node 1, which initially has the highest amount of heat, is directly connected to many other nodes whose heat contents are very low. Thus, node 1 plays a central role in the exchange of heat within its neighborhood. The neighboring nodes to node 1 which had no heat initially, steadily gain equal amounts of heat from node 1 and as such their heat content raises as time goes by until the equilibrium point is reached. At $t = 6$, the quantity of heat at all nodes is the same, that is, $\phi_j(6) = 1.6$ which implies equilibrium is attained for all nodes in the network.
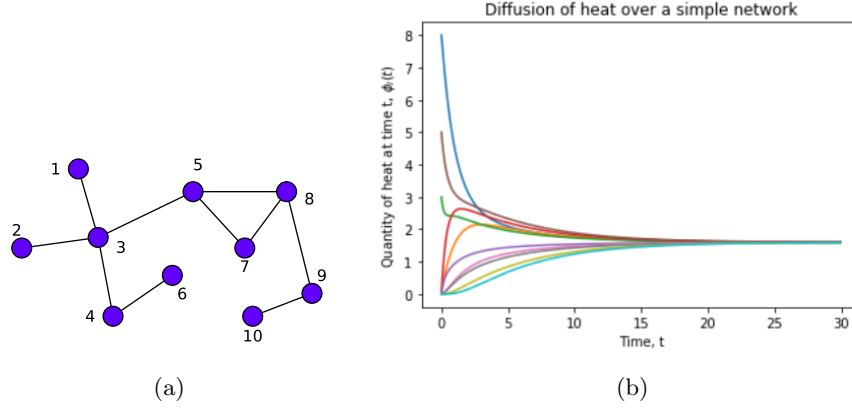
Figure 1: (b) is an illustration of the diffusion process over the network in (a).

For the 4-regular network shown in Fig. 3(a).Suppose we set initial heat quantities as in the star network and with the same diffusion constant,we illustrate the diffusion process by Fig. 3(b). We observe that diffusion occurs much faster than in the star network that is to say by $t = 2$, nodes are already tending to equilibrium point.
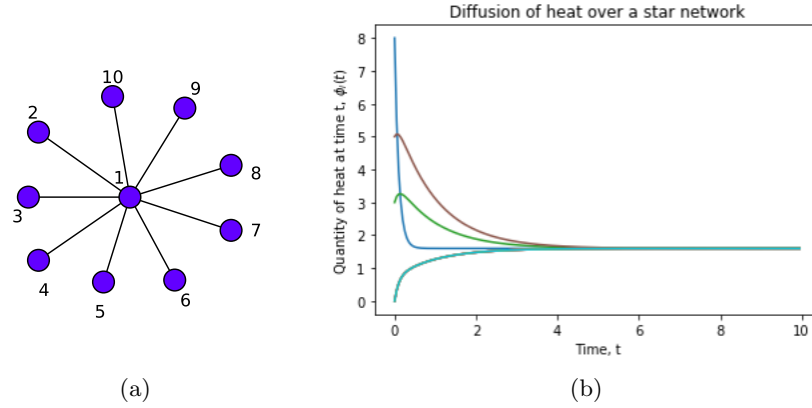


Figure 2: (b) is an illustration of the diffusion process over a star network in (a).
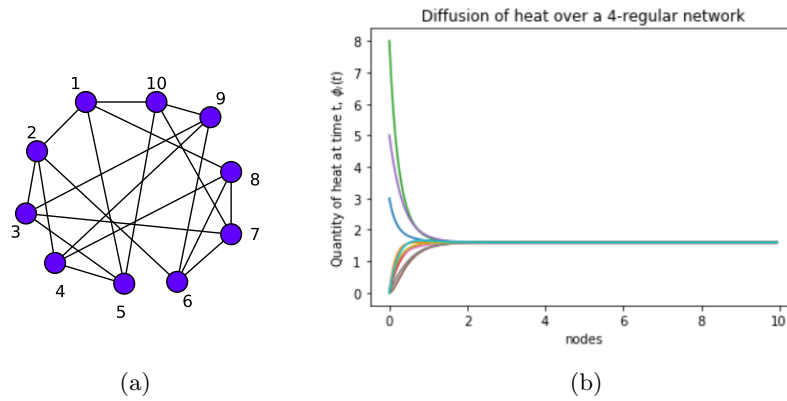


Figure 3: (b) is an illustration of the diffusion process over a 4-regular network in (a).

A better visualisation of the diffusion process over the network in Fig. 1(a) at different time intervals is illustrated in Fig. 4 where the quantity of heat at any node at time $t$ is proportional to the size of the node.
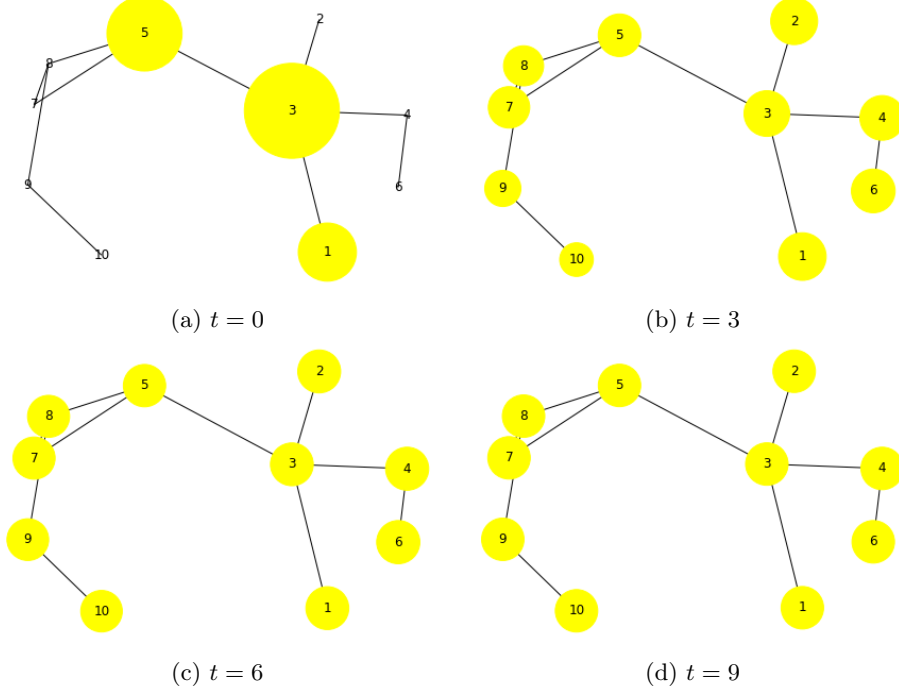
(a) $t = 0$        (b) $t = 3$

(c) $t = 6$        (d) $t = 9$

Figure 4: Illustration of the diffusion process on a simple network in Fig. 1(a). Initially(t=0), all nodes are assigned certain quantities of heat according to the vector $\phi_0 = [3, 0, 8, 0, 5, 2, 0, 0, 0, 2]$ where by the size of the node is proportional to the heat quantity that node has. Figures 4a, 4b, 4c, and 4d depict the status of the networks at $t = 1$, $t = 3$, $t = 6$, and $t = 9$ respectively.

In conclusion, we can tell that the structure of a network, the centralities of nodes, and the initial distribution of heat over a network play a key role in the diffusion process and hence have an impact on when diffusion is reached. For instance, equilibrium is reached faster in the star network as compared to the other two networks because the most central node of the star network (node 1) exchanges heat with its neighbors at a fast rate until equilibrium is reached.

# 4   Diffusion on network with long range interactions

In this case, we consider diffusion in a network where by both direct and long range interactions are involved. The long range interaction between two nodes $i$ and $j$ is determined by the length of the shortest path $d_{i,j}$ between nodes and the parameter $x$ ($0 \leq x < 0.5$). Thus, for any two that are not neighbours, we quantify long range interaction between them as $d_{i,j} x^{d_{i,j}-1}$. For a simple undirected network with $n$ nodes, In case we consider a generalised adjacency matrix $A_{ij}(x)$ given by

$$ A_{i,j}(x) = \begin{cases} 1 & \text{if} \quad i \sim j \\ d_{ij} x^{d_{ij}-1} & \text{if} \quad i \nsim j \quad \& \quad i \neq j \\ 0 & \text{if} \quad i = j, \end{cases} $$

where $d_{ij}$ is the shortest distance between nodes $i$ and $j$ and $x$ is referred to as the conductance such that $0 \leq x < 0.5$.

Taking into account both direct and long range interactions (introducing conductance $x$), the rate of

change in heat quantities for a given node $i$ over a change in time is given as

$$\frac{d\phi_i(x)}{dt} = C\sum_j A_{i,j}(x)(\phi_j - \phi_i)$$

$$\frac{d\phi_i(x)}{dt} = C\sum_j A_{i,j}(x)\phi_j - C\phi_i\sum_j A_{i,j}(x)$$

$$\frac{d\phi_i(x)}{dt} = C\sum_j A_{i,j}(x)\phi_j - C\phi_i k_i(x)$$

$$\frac{d\phi_i(x)}{dt} = C\sum_j (A_{i,j}(x) - \delta_{i,j}k_i(x))\phi_j$$

In matrix notation;

$$\frac{d\phi(x)}{dt} + CL(x)\phi(x) = 0, \quad \phi(0,x) = \phi(0) = \phi_0, \tag{11}$$

whose solution is

$$\phi(t,x) = \phi_0 \, e^{-CL(x)t}$$

On the other hand, the solution can be expressed as a linear combination of eigenvectors $v_i(x)$ of $L(x)$

$$\phi(t,x) = \sum_i a_i(t,x)v_i(x)$$

Substituting for $\phi_i(x)$ in 11, we have

$$\frac{da_i(t,x)}{dt} + C\lambda_i(x)a_i(x) = 0, \quad i = 1,\ldots,n.$$

whose solution is

$$a_i(t,x) = a_i(0,x)e^{-C\lambda_i(x)t} \tag{12}$$

Thus,

$$\phi(t,x) = \sum_i a_i(0,x) \, e^{-C\lambda_i(x)t}\mathbf{v_i(x)}$$

where

$$a_i(0,x) = \langle \phi(0), \mathbf{v_i(x)} \rangle$$

Therefore given eigenvalues of $L(x)$ and their corresponding eigenvectors along with the initial heat quantities at each node $\phi_0$, we can compute the quantity at each node at a particular time $t$.

As time tends to infinity, we can tell from eqn 12 that equilibrium behaviour can be attained because the eigenvalues of the laplacian matrix $L(x)$ at conductance $x$ are non negative values which implies that the solution to eqn 12 only decays exponentially or remains constant. However, it is important to note that rate of exponential decay is relatively faster when long range interactions are involved. This is because the eigenvalues $\lambda(x)$ are increasing functions of $x$ implying that $\lambda(x) \geq \lambda$. So we have

$$\lim_{t \longrightarrow \infty} e^{-C\lambda_i(x)t} = \begin{cases} 0 \text{ if } & \lambda_i(x) > 0 \\ 1 \text{ if } & \lambda_i(x) = 0 \end{cases}$$

This implies that for $\lim_{t \longrightarrow \infty}$, the solution to eqn 12 is $a_i(0,x)e^{-C\lambda_i(x)t}$ for $\lambda_i = 0$. In other words, the equilibrium state of the system is completely determined by the kernel ($ker(L(x)) = \{\mathbf{v} \in \mathbf{V} | \mathbf{L}(x,\mathbf{v}) = \mathbf{0}\}$) of the $L(x)$. One of the vectors in $ker(L(x))$ is the all ones vector $\mathbf{v^1}$ since $\sum_j L_{i,j}(x) = 0$.
So for a graph with $n$ nodes and initial heat quantities $phi_i$ at each node $i$, equilibrium behaviour is given by

$$\lim_{t \longrightarrow \infty} \phi(t,x) = \langle \phi_0, \mathbf{v(x)^1} \rangle \mathbf{v(x)^1}$$

The quantity of heat $\phi_j(t, x)$ at any node $j$ at time $t$ when $x$ is introduced is given by

$$\lim_{t \longrightarrow \infty} \phi_j(t, x) = \frac{1}{n} \sum_{i=1}^{n} \phi_i(0)$$

# 5 Diffusion with long range Interactions for different Network structures

Here we consider two networks that is Barabasi-Albert network whose degree distribution follows a power law and the other is the Erdos-Renyi network whose degree distribution follows exponential distribution. Both networks have 1000 nodes and average degree 6. We then investigate diffusion over the two networks for different values $x$ and results illustrated in Fig 5.

From Fig 5 at the top row, we observe that at $x = 0$, equilibrium is reached faster for Barabasi-Alberto(BA) network ( that is after about 4 time steps) compared to Erdos-Renyi(ER) network in which equilibrium is reached after about 10 time steps. This is explained based on the fact that in BA networks there are more hubs compared to ER networks. These hubs tend to interact with a number of nodes with in the network thus fastening the diffusion process. On increasing $x$ to 0.2, we observe a drastic drop in equilibrium time from 4 to 0.15 time steps and from 10 to 0.8 time steps for BA and ER networks respectively. It is important to note that drop in equilibrium time is relatively higher in ER than in BA and this is because of the few hubs in ER networks which aids a larger number of long range interactions than in BA networks. As $x$ increases further to 0.4, equilibrium time further drops to 0.03 and 0.06 for BA and ER networks respectively.

# 6 Degree Centrality and Diffusion on networks

We observe that in BA network, heat spreads quite faster than in ER network that is to say by $t = 0.6$, all the 5 hubs in BA have levelled to equal amount while for ER, nodes still have un equal amounts of heat. This is because we assign quantities of heat to 5 hubs of a network and they quickly spread heat to other nodes compared to ER where there are relatively fewer hubs among the five chosen nodes to initiate the diffusion process.

# 7 Diffusion process on a grid

We consider a 2-dimensional discrete grid in which each point is connected to 8 of its nearest neighbours. Initially, we assign heat quantities to all the points on the grid and then we investigate how the diffusion process occurs and at each time $t$, we compute the quantity of heat at each node using equation 2.
Let us take a 20 by 20 grid on which we assigned heat quantities of amounts 5, 7 and 10 to a few points and the rest are assigned zero. The figures below illustrate the diffusion process in which both the direct and long range interactions are accounted for at different values of x.

At $t = 0$, diffusion on the grid starts off with 3 strong regions having high quantities of heat as observed from observe figures ??, 10, and ?? which correspond to $x$ values of 0, 0.1 and 0.2 respectively. As the diffusion process continues, we see that at $t = 0.5$, strong heat points can still be spotted for $x = 0$, relatively strong points in $x = 0.1$ and almost complete diffusion in $x = 0.2$. we can also see that by $t = 2.0$, heat is uniformly distributed across the grid for $x = 0.1$ and $x = 0.2$. However, for $x = 0$ diffusion is still ongoing and we can notice strong heat points at the centre of the grid. Following the sequences in the figures, we can conclude that as $x$ (i.e increase in intensity of long range interactions), the diffusion process goes faster and equilibrium across the grid is reached faster as observed in the above simulations where for $x = 0.2$, $x = 0.1$ equilibrium is reached by $t = 3$ while for $x = 0$, equilibrium is not yet reached by then.

(a) $x = 0$           (b) $x = 0$

(c) $x = 0.2$           (d) $x = 0.2$

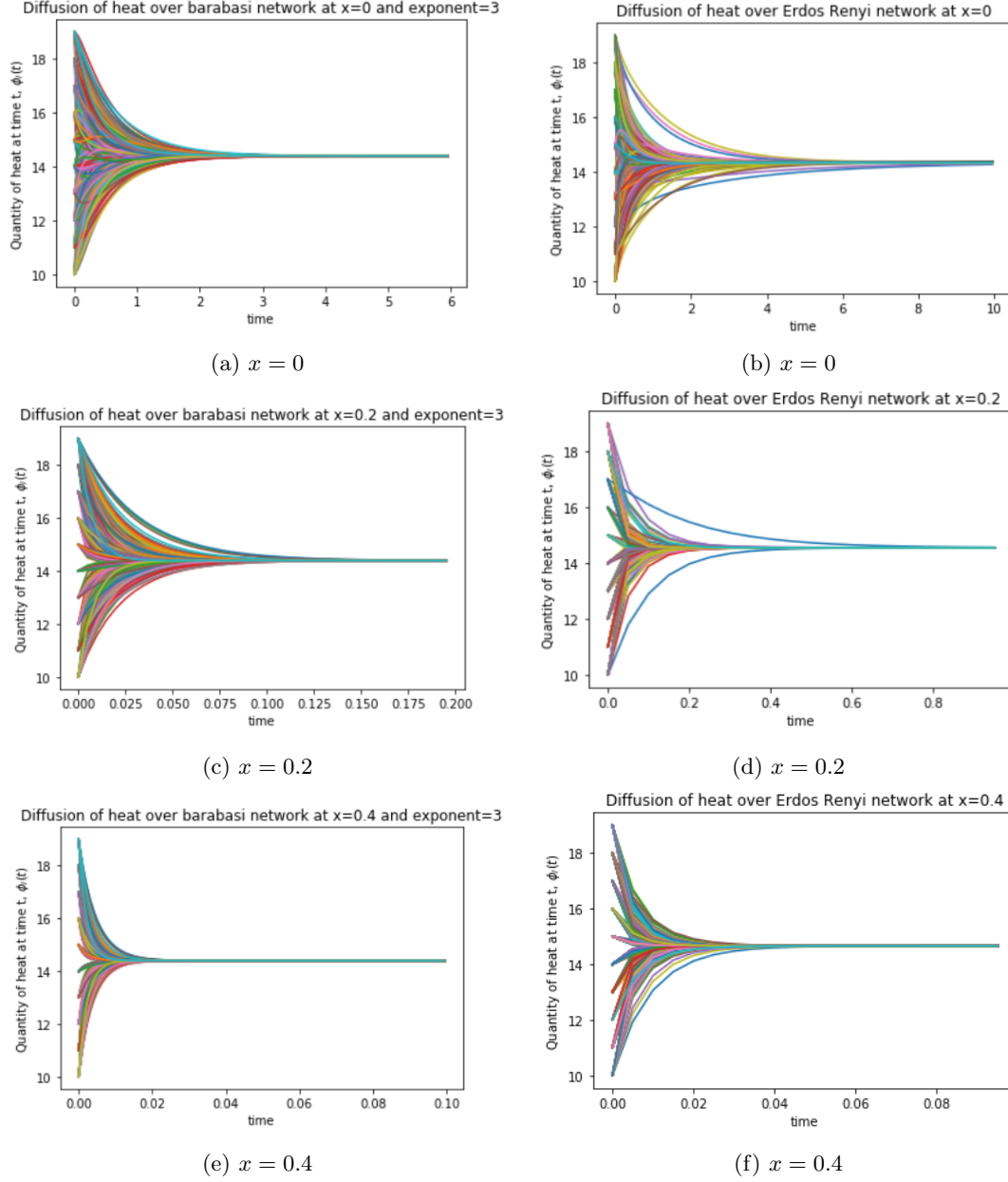(e) $x = 0.4$           (f) $x = 0.4$

Figure 5: Barabasi networks (left) and Erdos Renyi networks(right) of 1000 nodes and average degree of 6. Top row is illustration of diffusion process at $x = 0$ ( i.e accounting for direct interactions only), middle row corresponds to $x = 0.2$ followed by $x = 0.4$ in the last row
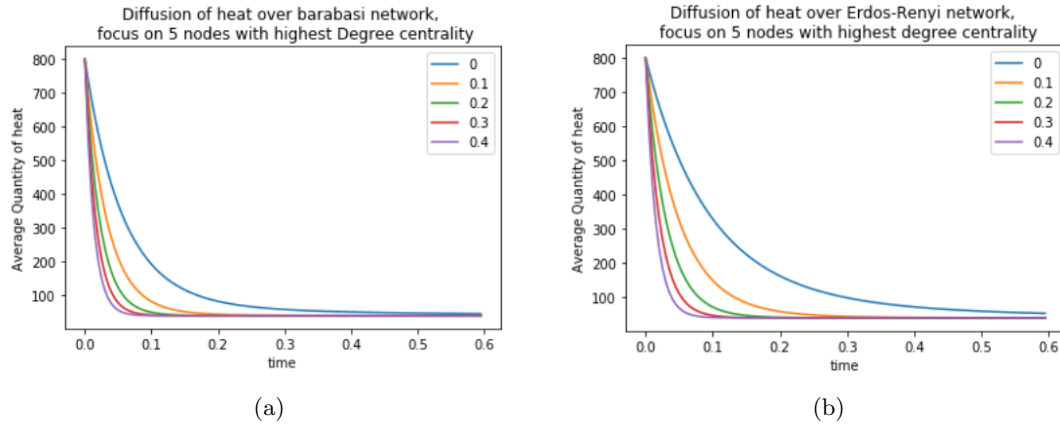
# 8 Previous Discussions

Figure 6: Results of the simulations for two networks. One is the Barabasi-Albert(BA) network and the other is Erdos-Renyi(ER) network, both of 100 nodes and average degree of 6. Taking 5 of the most important (by degree) nodes in the network from which diffusion is initiated by assigning certain quantities of heat to those nodes, the simulation of the diffusion is illustrated in plots (a) and (b) for the BA and ER networks respectively.
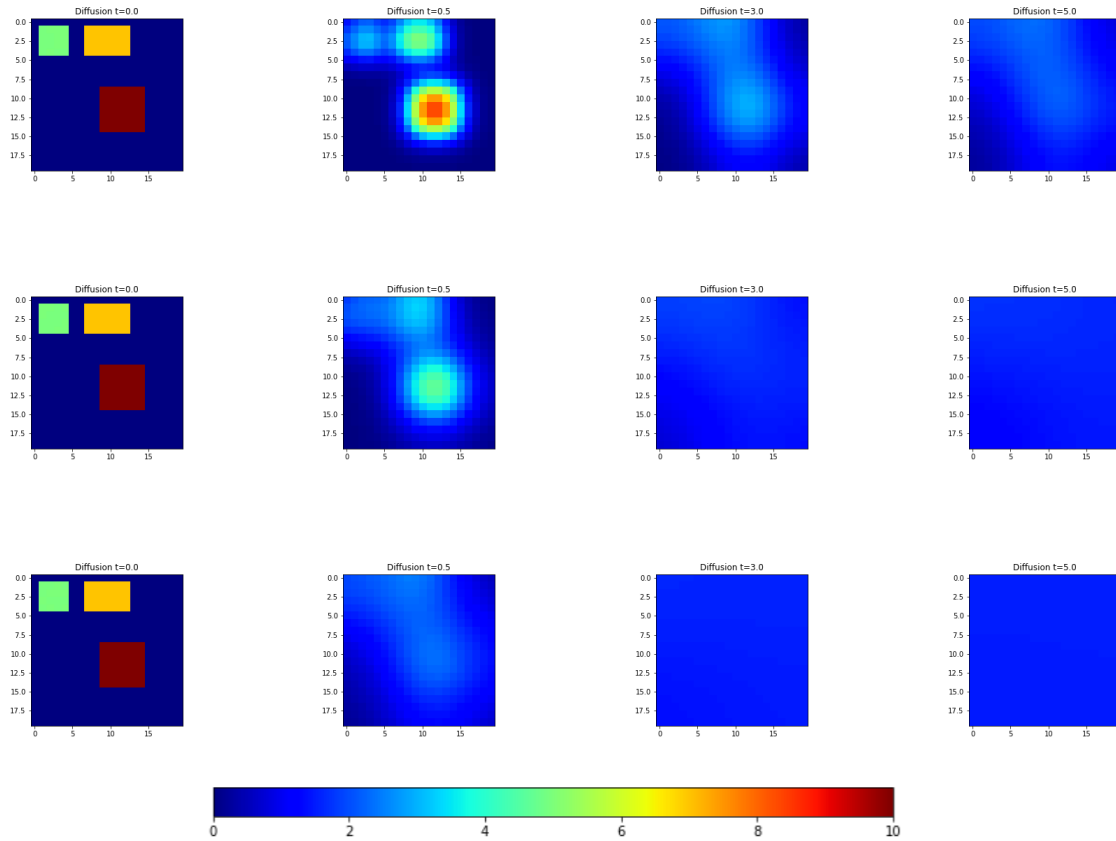


Figure 9: Illustrations for diffusion over a grid. The upper most row corresponds to diffusion when only direct interac tions among neighbouring nodes are accounted for. The middle and last row are results obtained when long range interactions are included at $x = 0.1$ and $x = 0.2$ respectively. The intensity of heat follows a color grid where by red implies higher intensity followed by yellow and blue implies low heat intensities.
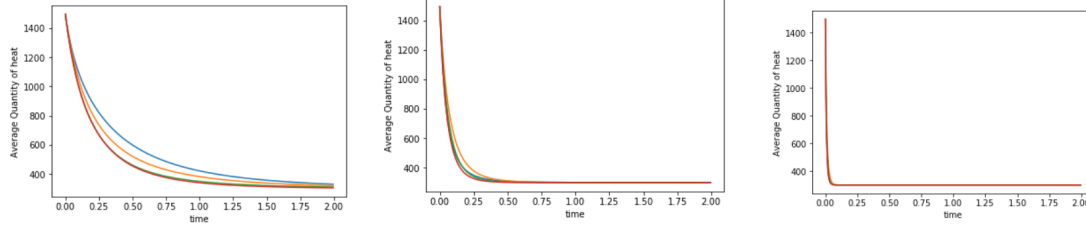
Figure 10: Plots of the average quantity of heat for 200 nodes with the highest degree centrality against time for 3 scale free networks having different values of the power exponent(2.0,2.3,2.7, and 3.0), n=1000 and average degree=6. The figures to the left, centre and right correspond to x values 0,0.1, and 0.3 respectively.
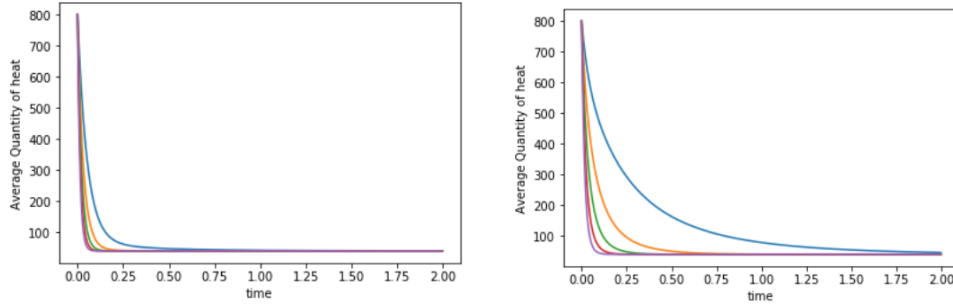


Figure 11: Illustration of the impact of the choice of the initial nodes from which diffusion starts. We consider Barabasi-Alberto networks of 100 nodes. The left plot corresponds to one in which the 5 most important node according to degree centrality(hubs) are chosen. On the other hand, the right plot is as a result of choosing the initial nodes randomly.
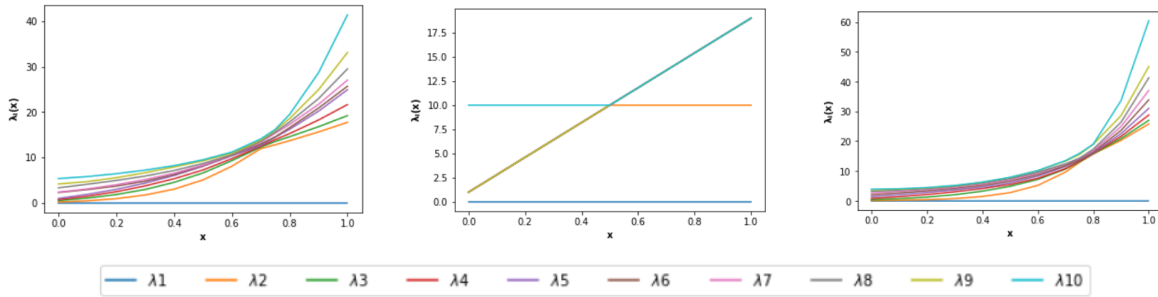


Figure 12: Results showing variation of eigenvalues with $x$. From left to right is simple networks(Fig. 1a), star network (in Fig. 2a) and path network respectively. All networks consist of 10 nodes.

# References

[1] A. Barrat, M. Barthelemy, R. Pastor-Satorras, and A. Vespignani. The architecture of complex weighted networks. *Proceedings of the National Academy of Sciences of the United States of America*, 101(11):3747–3752, 2004.

[2] M. Belkin and P. Niyogi. Laplacian eigenmaps for dimensionality reduction and data representation. *Neural computation*, 15(6):1373–1396, 2003.

[3] K. C. Das. The laplacian spectrum of a graph. *Computers & Mathematics with Applications*, 48(5):715–724, 2004.

[4] C. H. Edwards and D. E. Penney. *Differential equations and boundary value problems*, volume 2. Prentice Hall, 2004.

[5] E. Estrada. *The structure of complex networks: theory and applications*. OUP Oxford, 2011.

[6] E. Estrada. Path laplacian matrices: introduction and application to the analysis of consensus in networks. *Linear Algebra and its Applications*, 436(9):3373–3391, 2012.

[7] E. Estrada. Introduction to complex networks: structure and dynamics. In *Evolutionary Equations with Applications in Natural Sciences*, pages 93–131. Springer, 2015.

[8] E. Estrada, F. Kalala-Mutombo, and A. Valverde-Colmeiro. Epidemic spreading in networks with nonrandom long-range interactions. *Physical Review E*, 84(3):036110, 2011.

[9] E. Estrada, P. Knight, et al. *A first course in network theory*. Oxford University Press, USA, 2015.

[10] E. Estrada and J. A. Rodriguez-Velazquez. Subgraph centrality in complex networks. *Physical Review E*, 71(5):056103, 2005.

[11] L. Euler. Leonhard euler and the königsberg bridges. *Scientific American*, 189(1):66–70, 1953.

[12] J. Gower. A modified leverrier-faddeev algorithm for matrices with multiple eigenvalues. *Linear Algebra and its Applications*, 31:61–70, 1980.

[13] I. Gribkovskaia, Ø. Halskau, and G. Laporte. The bridges of königsbergâa historical perspective. *Networks*, 49(3):199–203, 2007.

[14] I. Gutman and O. E. Polansky. *Mathematical concepts in organic chemistry*. Springer Science & Business Media, 2012.

[15] J. M. Harris, J. L. Hirst, and M. J. Mossinghoff. *Combinatorics and graph theory*, volume 2. Springer, 2008.

[16] Internet. Network. [Online; accessed 2016-03-29].

[17] R. Kasprzak. Diffusion in networks. *Journal of Telecommunications and Information Technology*, pages 99–106, 2012.

[18] R. Kondor and J.-P. Vert. Diffusion kernels. *kernel methods in computational biology*, pages 171–192, 2004.

[19] J. Lafferty and G. Lebanon. Diffusion kernels on statistical manifolds. *Journal of Machine Learning Research*, 6(Jan):129–163, 2005.

[20] D. López-Pintado. Diffusion in complex social networks. *Games and Economic Behavior*, 62(2):573–590, 2008.

[21] H. Ma, H. Yang, M. R. Lyu, and I. King. Mining social networks using heat diffusion processes for marketing candidates selection. In *Proceedings of the 17th ACM conference on Information and knowledge management*, pages 233–242. ACM, 2008.

[22] S. Milgram. The small world problem. *Psychology today*, 2(1):60–67, 1967.

[23] J. J. Molitierno. *Applications of combinatorial matrix theory to Laplacian matrices of graphs*. CRC Press, 2012.

[24] F. K. Mutombo. *Long-range interactions in complex networks*. PhD thesis, University of Strathclyde, 2012.

[25] M. Newman. *Networks: an introduction*. OUP Oxford, 2010.

[26] M. E. Newman. Scientific collaboration networks. ii. shortest paths, weighted networks, and centrality. *Physical review E*, 64(1):016132, 2001.

[27] Nexus. Zachary's karate club [karate], 2012. [Online; accessed 2016-04-25].

[28] T. Opsahl. *Structure and evolution of weighted networks*. PhD thesis, Queen Mary, University of London, 2009.

[29] T. Opsahl, F. Agneessens, and J. Skvoretz. Node centrality in weighted networks: Generalizing degree and shortest paths. *Social Networks*, 32(3):245–251, 2010.

[30] T. Opsahl and P. Panzarasa. Clustering in weighted networks. *Social networks*, 31(2):155–163, 2009.

[31] X. Qi, R. D. Duval, K. Christensen, E. Fuller, A. Spahiu, Q. Wu, Y. Wu, W. Tang, C. Zhang, et al. Terrorist networks, network energy and node removal: a new measure of centrality based on laplacian energy. *Social Networking*, 2(01):19, 2013.

[32] X. Qi, E. Fuller, Q. Wu, Y. Wu, and C.-Q. Zhang. Laplacian centrality: A new centrality measure for weighted networks. *Information Sciences*, 194:240–253, 2012.

[33] X. F. Wang and G. Chen. Complex networks: small-world, scale-free and beyond. *Circuits and Systems Magazine, IEEE*, 3(1):6–20, 2003.

[34] D. J. Watts and S. H. Strogatz. Collective dynamics of âsmall-worldânetworks. *nature*, 393(6684):440–442, 1998.

[35] R. J. Wilson. *An introduction to graph theory*. Pearson Education India, 1970.