School of Mathematical Sciences

Properties of perturbed lattices

Author:
Yue Wu

Supervisor:
Dr Anna V. Maltsev

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Contents

Abstract

This study focuses on perturbed lattice geometric graphs (PLGG). Perturbed lattices refer to lattices with random deviations in position. PLGG are graphs which begin with a set of perturbed lattices and connect nodes with a connection function that takes distance as a parameter. In this study, we look at both "hard" and "soft" PLGG, distinguished by their connection functions. The study examines various key properties of both models, including the fraction of nodes in the largest component, connectivity, degree distribution, and spectral properties. The main result of this study is that the effect of disorder on the largest component is reversed in the hard and soft graphs. The degree distribution and spectral properties of the graphs are also studied. The study aims to build an idealized model for the Spontaneous calcium release (SCR) found in cardiac cells and provides a reference when modelling cellular networks with repulsion.

1 Introduction

1.1 Background

Geometric graphs (GG) are graphs starting with a set of vertices in a space, normally two- or three-dimensional Euclidean space. Nodes will be connected if their distance is less than the given connection radius r. This study focuses on perturbed lattice geometric graphs (PLGG), that is, GG start with a perturbed square lattice. We also look at the case instead of connecting any two nodes within a certain range to each other but connecting them with a probability function that takes distance as a parameter (soft PLGG). In the following text, we will refer to them as "hard graph" and "soft graph" based on their connection functions. We studied various key properties of both models, such as the fraction of nodes in the largest component, connectivity, degree distribution and various spectral properties.

Graphs are often used for modelling the relationship of units within complex systems. In order to extract interesting information efficiently that is hidden in the real world, past researchers have introduced many random graph models. The Erdős–Rényi G(n,p) model is the earliest proposed random graph model where every pair of nodes is connected with a fixed probability $p \in (0,1)$ [1]. Another widely used model is Barabasi and Albert scale-free networks which have broad degree distribution with diverging $\langle k^2 \rangle$ and perform good simulation for many systems such as the WorldWide-Web and the citation networks [2]. Many random graph models are introduced by considering primarily their general properties. However, for many complex networks, the underlying spatial structure is an important property, and the geometry can significantly impact the network's topology [3]. RGG is one of the most commonly used models that incorporate spatial information [4].

RGG was first introduced to model the communications between radio stations and become a popular research topic nowadays. The applicability of RGG has been widely confirmed. In 2003, RGG was used to study degree distribution in wireless ad-hoc networks [5]. The results presented here are useful of connectivity and estimation of the capacity in ad-hoc networks. By taking diversities of research contents between papers as distance, RGG was used to model citation network in [6]. The abundance of triangles in an RGG is the fundamental difference between RGG and other models that makes analysis challenging for RGG.

The driving motivation of this study comes from a recent paper about Spontaneous calcium release (SCR) [7]. Ca spark refers to Ca release from the sarcoplasmic reticulum (SR) by several thousand Ca-releasing units (CRUs) [8]. SCR refers to under conditions such as Ca overload, the Ca released during a spark can also diffuse and induce Ca sparks in neighbouring CRUs. This chain reaction of events can lead to Ca waves propagating across the cell, leading to a substantial depletion of Ca from the SR [9]. Excessive SCR is a phenomenon recognised as a cause of cardiac arrhythmias [10]. It was found that the spatial disorder among the CRUs aids calcium wave propagation [7]. We aim to build an idealised model for this phenomenon where complex parameters such as calcium diffusion and cellular electrophysiology. Besides that, a study of PLGG can also provide a reference when modelling cellular networks with repulsion.

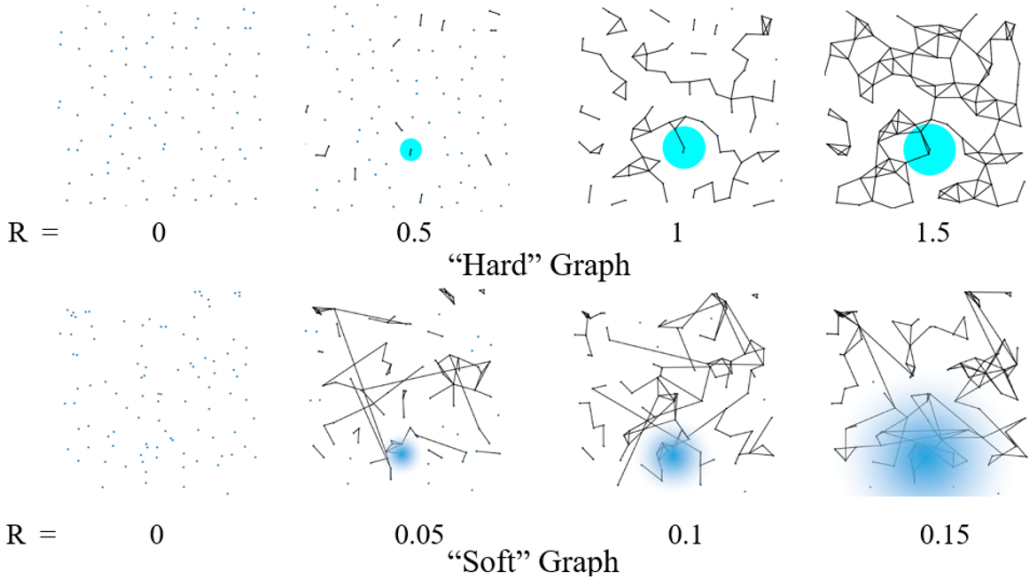


Figure 1: Random geometric graphs for different connectivity parameters r.

Through numerical analysis and modelling using Python, we found that the effect of disorder on the size largest component is reversed in hard and soft graphs. The exact degree distribution of the model is obtained. Furthermore, the spectral properties of the graph were explored, and we found that the principle eigenvalue and the mean degree of the graph showed a strong correlation.

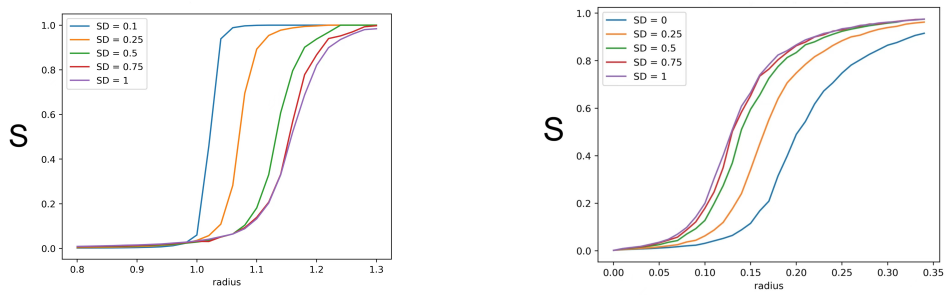
1.2 Model construction

Our PLGG consists of two parameters, standard deviation σ that indicates randomness and connection radius R. The model starts with a rectangular lattice on a torus. Then, we add an independent identically distributed Gaussian random variable for each vertex with mean 0 and standard deviation σ on both the x and y-axis. In "hard" graphs, any two vertices are connected if the Euclidean distance between them is less than the connection parameter R. In the "soft" graph, first define connection function $C(D,R)$: $\mathbb{R}_+ \to [0,1]$, then connect any two vertices with probability C (See Figure 1.), in this study, the connection function of "soft" graph is $C(D,R) = \min\left\{1, \frac{R}{D^3}\right\}$.

2 General properties of PLGG

2.1 Largest component and percolation

A graph's connected component is a sub-graph in which every vertex is linked to each other by paths. The largest connected component is the connected component with the maximum number of vertices. The fraction of nodes in the largest connected component reveals the percolation properties. Percolation describes the behaviour of a graph when certain vertex or links are added, small, disconnected components merge into



(a) (b)

Figure 2: Plot of average fraction of nodes S in the largest component versus radius of "hard" graph (a) and "soft" graph (b) from 100 simulations, each line corresponds to a different standard deviation where the blue line represents the least disordered lattice and the purple line represents the most disordered lattice.

significantly larger connected components. In order to explore what is the impact of the disorder on percolation, we simulate the graph and then compute the size of the largest component in the simulation (See Figure 2.) Although we do not observe a sharp threshold for phase transition in hard and soft graphs, we found that the disorder's impact plays a different role in our models. For hard graphs, disorder impedes percolation, increase in standard deviation right shifts the curve. However, for soft graphs, the opposite effect occurs, the disorder aids percolation.

2.2 Degree distribution

In previous study done by Dr. Maltsev, the exact formula for degree distribution was derived. In the following section, I will provide a simplified version of the proof. For any two vertex on the lattice V_1 and V_2, the difference between their x coordinates $x_1 - x_2$ where x_1, x_2 are starting x coordinates of V_1, V_2. By perturb them, we added Gaussian number with $\mu = 0$ and standard deviation $= \sigma$ to x coordinates of each nodes. Thus, difference of x coordinates between two nodes in perturbed lattice are random variables follows Gaussian distribution with $\mu = x_1 - x_2$ and variance = $2\sigma^2$, denote as X. Similarly, difference of y coordinates Y follows Gaussian distribution with $\mu = y_1 - y_2$ and variance = $2\sigma^2$. To connect two vertex, we need distance D between them be less than connection radius R that is

$$\begin{aligned}
\mathbb{P}(D < R) &= \mathbb{P}(\sqrt{X^2+Y^2} < R) \\
&= \mathbb{P}(X^2+Y^2 < R^2) \\
&= \mathbb{P}(\frac{X^2}{2\sigma^2} + \frac{Y^2}{2\sigma^2} < \frac{R^2}{2\sigma^2}) \\
&= P(R, X^2+Y^2, \sigma).
\end{aligned}$$

Notice that $\frac{X}{\sqrt{2}\sigma}$ and $\frac{Y}{\sqrt{2}\sigma}$ are independent Gaussian distributed variables with unit variance. By definition of non-central chi square distribution, $\frac{X^2}{2\sigma^2} + \frac{Y^2}{2\sigma^2}$ follows non-

central chi square distribution with degree of freedom = 2, and non-centrality parameter $\lambda = X^2 + Y^2$. Using P.D.F of non-central chi square distribution we obtain

$$P(R,\lambda,\sigma) = \frac{1}{2}\int_0^{\frac{R^2}{2\sigma^2}} e^{-\frac{1}{2}\left(t+\frac{\lambda}{2\sigma^2}\right)} I_0\left(\frac{\sqrt{\lambda t}}{\sqrt{2}\sigma}\right) dt, \tag{1}$$

where I_0 is the modified Bessel function of the first kind, $\lambda = X^2 + Y^2$. The degree distribution of a graph is a probability distribution that describes the frequency of nodes in the network with a given degree. To find the degree distribution, we only focus on vertex at (0,0). This is valid because the equations for all the vertices only depend on the distances between them and not their exact location. For each pair of vertex, there is probability of connected is $P(R,\lambda,\sigma)$ and probability of $1 - P(R,\lambda,\sigma)$ that there is not connected. Letting $B(a)$ be a Bernoulli random variable, Λ be the set of vertex, the degree distribution is given by

$$K = \sum_{(x,y)\in\Lambda\setminus(0,0)} B\left(P\left(R, x^2+y^2, \sigma\right)\right). \tag{2}$$

Therefore, mean of degree distribution is

$$\langle K\rangle = \sum_{(x,y)\in\Lambda\setminus(0,0)} P\left(R, x^2+y^2, \sigma\right). \tag{3}$$

For "soft" graph, we connect two nodes with $C(D,R) = \min\left\{1, \frac{R}{D^3}\right\}$. When $\frac{R}{D^3} \geq 1$, connections are bound to occur. Hence we have

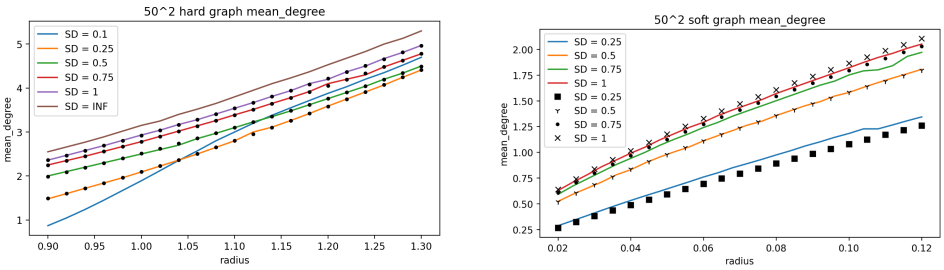
$$\mathbb{P}(V_1 \textit{ connects } V_2) = \mathbb{P}(D < R^{\frac{1}{3}}) + \mathbb{P}((U < \frac{R}{D^3}) \cap (D > R^{\frac{1}{3}}))$$

, Where $\mathbb{P}(D < R^{\frac{1}{3}})$ is simply $P(R^{\frac{1}{3}},\lambda,\sigma)$, for the LHS, we have

$$\begin{aligned}\mathbb{P}((U < \frac{R}{D^3}) \cap (D > R^{\frac{1}{3}})) &= \mathbb{P}(U < \frac{R}{D^3})\mathbb{P}(D > R^{\frac{1}{3}}) \\ &= \frac{R}{D^3}\mathbb{E}(\mathbf{1}_{D>R^{\frac{1}{3}}}),\end{aligned}$$

where $\mathbf{1}_{D>R^{\frac{1}{3}}}$ is the activate function that outputs 1 when the condition $(D > R^{\frac{1}{3}})$ mets and outputs 0 when condition fails. Let $Q(R^{1/3},\lambda,\sigma)$ be the LHS probability. Using the same variance normalization used above, the expectation of activation function can be find

$$\begin{aligned}Q(R^{1/3},\lambda,\sigma) &= R(\sqrt{2}\sigma)^{-3}\mathbb{E}\frac{1\left(\frac{X}{\sqrt{2}\sigma}\right)^2 + \left(\frac{Y}{\sqrt{2}\sigma}\right)^2 > \frac{R^2/3}{2\sigma^2}}{\left(\left(\frac{X}{\sqrt{2}\sigma}\right)^2 + \left(\frac{Y}{\sqrt{2}\sigma}\right)^2\right)^{3/2}} \\ &= \frac{R}{2^{5/2}\sigma^3}\int_{\frac{R^2/3}{2\sigma^2}}^{\infty} t^{-3/2} e^{-\frac{1}{2}\left(t+\frac{\lambda}{2\sigma^2}\right)} I_0\left(\frac{\sqrt{\lambda t}}{\sqrt{2}\sigma}\right) dt.\end{aligned} \tag{4}$$



(a) (b)

Figure 3: Plot of mean degree versus radius of "hard" graph (a) and "soft" graph (b) from 100 simulations. The lines are the mean values of the simulations and the points are the analytical solutions.

Hence, we obtained degree distribution

$$K_{\text{soft}} = \sum_{(x,y)\in\Lambda\setminus(0,0)} B\left(P\left(R^{1/3},\lambda,\sigma\right)+Q\left(R^{1/3},\lambda,\sigma\right)\right), \tag{5}$$

and mean of degree distribution

$$\langle K_{\text{soft}}\rangle = \sum_{(x,y)\in\Lambda\setminus(0,0)} P\left(R^{1/3},x^2+y^2,\sigma\right)+Q\left(R^{1/3},x^2+y^2,\sigma\right). \tag{6}$$

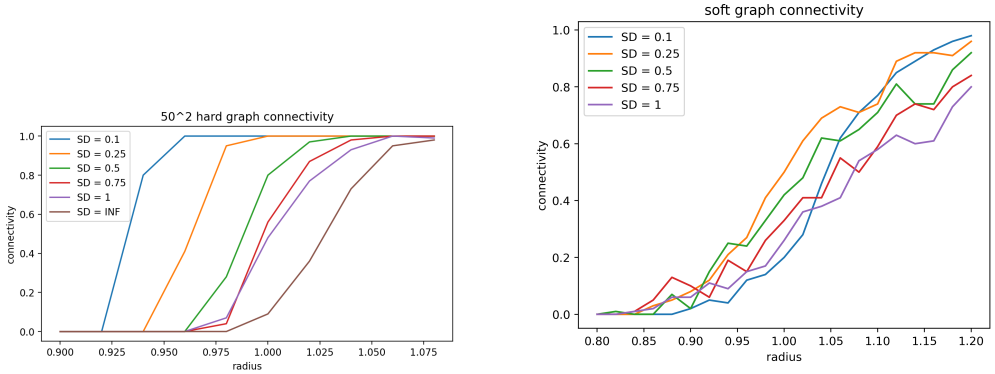
To check formula (3) and (6), we compared numerical result and average mean degree of simulation (See Figure 3.)

2.3 Connectivity

In graph theory, a connected graph consists of one component without any isolated vertex. In other words, there are paths between every pair of vertex. In this study, connectivity is defined as the probability of getting a full connected graph. We aim to find how the change of parameters would affect the connectivity of PLGG. Figure 4. presents the observed connectivity of PLGG with 100 simulation runs. In "hard" graph (Figure 4 (a)), the threshold for connectivity growth increases as the standard deviation increases, and there is a slight slowdown in the rate of connectivity growth. Disorder in the lattice impedes connectivity. In the "soft" graph (Figure 4 (b)), the effect of disorder in the lattice is much smaller, and connectivity does not increase explosively but steadily.

3 Spectral properties of PLGG

In graph theory, spectral properties are about eigenvalues and eigenvectors of the adjacency matrix or Laplacian matrix. In the following section, we studied the relationship between the mean degree and leading eigenvalue of the adjacency matrix and gave a method for predicting the leading eigenvalue. Furthermore, we studied the properties of the leading eigenvector.



(a) (b)

Figure 4: Plot of mean degree versus radius of "hard" graph (a) and "soft" graph (b) from 100 simulations. The lines are the mean values of the simulations and the points are the analytical solutions.

3.1 Leading eigenvalue and average degree

For a graph, the average degree is bounded by its adjacency matrix's leading eigenvalue. Let A be the adjacency matrix of PLGG with n nodes, λ_1 be the leading eigenvalue (LEV) of A, Rayleigh quotient gives

$$\lambda_1 = \max_x \frac{x^T A x}{x^T x},$$

where $x \in \mathbb{R}^n$, hence

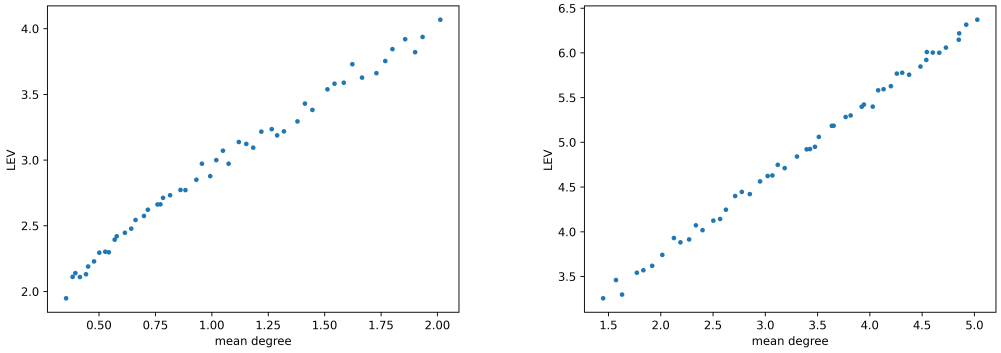
$$\lambda_1 \geq \frac{1^T A 1}{1^T 1} = \frac{\sum_{i,j} A(i,j)}{n} = \overline{d}. \tag{7}$$

Since we already obtained the exact formula for the mean degree, this gives us the range of LEV. In 2016, Estrada et al. found that LEV and the average degree are highly linearly correlated in RGG within rectangles [11]. This leads us to speculate whether the same relationship occurs with our model. Figure 5. is the scatter plot of the LEV versus the average degree for "hard" graphs (a) and "soft" graphs (b). We can observe that they are positively correlated. To better predict the LEV, we performed a linear regression analysis on the data.

σ	0.5	0.75	1
β_1	3.992	1.927	1.863
β_0	1.896	1.402	1.3623
R^2	0.960	0.998	0.990

Table 1: Results of linear regression analysis on hard graph

The linear model used is $\lambda_1 = \beta_0 * \overline{d} + \beta_1$. Table 1 and 2 shows the result of the linear fit. In linear regression, R^2 refers to the coefficient of determination. It is a scale-free one-number summary of the strength of the relationship between independent variables and dependent variables [12]. To be more precise, it measures the proportion of the variation



(a) (b)

Figure 5: Scatter plots of the leading eigenvalue of adjacency matrix versus the average degree for hard graph (a) and soft graph (b) for different values of the connection radius and $\sigma = 0.5$.

σ	0.5	0.75	1
β_1	1.983	2.320	2.506
β_0	0.871	0.915	0.962
R^2	0.997	0.994	0.993

Table 2: Results of linear regression analysis on soft graph

in the dependent variable that is predictable from the independent variables [13]. Tables I and II contain the linear fit for both plots, and it can be seen that in both plots, the value of R^2 is greater than 0.95, i.e. for more than 95% of the data being explained by the fitted line, regardless of how the standard deviation is changed. At the same time, as the standard deviation rises, both β_0 and β_1 drop with it in hard graphs. In "soft" graphs, opposite effects occur again, β_0 and β_1 increase with θ. Due to the difficulty of mathematical derivation of λ_1, this study does not give a method for direct prediction of the leading eigenvalue. However, we found a close linear relationship between the leading eigenvalue and the average degree, which we can compute analytically. In the next section, we will give one use of this finding.

3.2 Epidemic in a network

The spreading of infectious disease on networks can be modelled by representing individuals as nodes and the contacts between them as edges [11]. The susceptible Infected Susceptible (SIS) and Susceptible Infected Recovered (SIR) models are among the most widely known models. In the SIS model, each node must be in one of the following two states: susceptible (S) or infected (I). In the SIR model, there is an extra state for node: recovered (R). The difference between the two models is that SIS is used to simulate situations when repeated infections are possible, such as covid-19, while SIR is used to simulate the transmission of diseases that do not reproduce, such as chickenpox. Both models are governed by parameters, rate of infection β and recovery rate μ.

In general, we are interested in whether a disease will become an epidemic or dies

out after a small transmission period. In the SIS and SIR models, the rate of epidemic spreading τ is defined as

$$\tau = \frac{\beta}{\mu},$$

and there exits critical value of τ, i.e., epidemic threshold τ_c such that when $\tau_c \geq \tau$ pandemic dies and when $\tau_c < \tau$ there would be a epidemic [14]. In 2008, Van et al. proved that the epidemic threshold is closely related to spectral radius of adjacent matrix [15], where

$$\tau_c = \frac{1}{\lambda_1}, \tag{8}$$

according to the inequality (7), the epidemic threshold is bounded by

$$\tau_c \leq \frac{1}{\overline{d}}, \tag{9}$$

Since we have found that the leading eigenvalue and the mean degree are closely correlated, and we hold the exact formula for the mean degree, this allows us to closely estimate the epidemic threshold. In section 2.2, we speculate that in both types of PLGG, the mean degree rises with standard deviation. We hypothesize that when using hard graphs for disease transmission simulations, such as simulating the spread of disease between plants, the more random the location between units, the smaller the epidemic threshold is. In contrast, when using soft graphs, the impact of disorder is smaller.

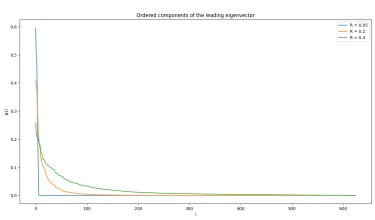
4 Maximum Degree

Studying the maximum degree of a graph can provide valuable insights into its properties. In the next section, we try to explore the nature of the maximum degree in PLGG and find the relationship between the leading eigenvector and the maximum degree.

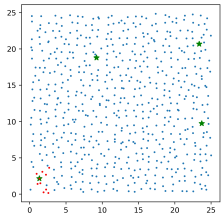
4.1 Leading eigenvector localization

Centrality in graph theory or complex networks is a concept that measures the importance of a node. Depending on how the importance of a node is measured, past scholars have defined many different kinds of centrality. For example, degree centrality counts the number of edges of nodes and betweenness centrality that measures how much a node acts as a bridge or intermediary between two closely related groups within a network. Eigenvector centrality (EC) is defined as the component of the principle eigenvector (PEV) associated with the leading eigenvalue of the adjacency matrix [16]. A node's EC is proportional to the sum of the EC scores of its neighbouring nodes [17]. Nodes connected to important nodes are more important. Nodes with a small number of influential contacts are likely to score higher EC than nodes with a large number of unnecessary contacts.

When the weight of the normalised leading eigenvector is concentrated on a small set of nodes, the leading eigenvector is localised. Pastor-Satorras and Castellano showed that in modelling epidemic spreading, the sub-graph in which the PEV is localised is



(a)



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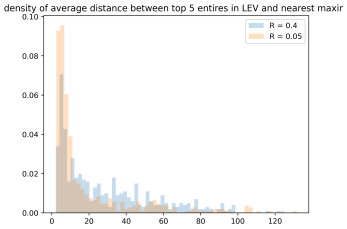

(c)

Figure 6: (a) Ordered components of the leading eigenvector ϕ_1, with elements normalized so that the maximum is 1. (b) Visualization of a soft graph where green star indicates nodes with highest degree centrality and red nodes are locations of top 10 entries of leading eigenvector. (c) Frequency for average distance between top 5 entries of leading eigenvalue and their nearest maximum degree.

the activation set of epidemic spreading (See [18]). In [19], the authors show that the location of the localised leading eigenvector appears around the nucleation site of a calcium wave. In this study, we're interested in the relationship between the location of the maximum degree and the localization location of the leading eigenvector. For the soft graph, we found the PEVs under different connection radius, normalised them and sorted them downwards (Figure 6 (a)). It can be noticed that a strong localisation feature appears in the PEV, which diminishes as the graph becomes more connected. Figure 6 (b) presents the top 10 entries and the node with the maximum degree (red node and green star, respectively). In this particular graph, the top 10 entries are clustered around the green star. To further verify the relationship between maximum degree and PEV localisation, the frequency for the average distance between the top 5 entries of leading eigenvalue and their nearest maximum degree is counted (See Figure 6 (c)). We conclude that most of the time, the PEV predicts the position of the maximum degree well, but this prediction can sometimes be wrong, and the accuracy of the prediction decreases as the graph becomes more connected (increase in radius).

5 Discussion and conclusion

In this study, we investigate the fundamental properties of PLGG through simulations in Python and numerical analysis. We find that in the "hard" graph, the stronger the lattice is perturbed, the larger the connection radius required to form the giant component, while in the "soft" graph, the stronger the lattice is perturbed, the smaller the connection radius required to form the giant component. Furthermore, we found a linear relation-

ship between the mean degree and the principal eigenvalue. We also found that the leading eigenvectors are highly localised, and the entries with high weight are concentrated around the maximum degree. In addition, we found the distribution of the maximum of n identically and independently distributed random variables (See Appendix). We plan to find an analytical solution for the maximum degree in future studies. The fact that the degrees of the nodes were not independent of each other makes it hard. Therefore, we assume the degree of independence of nodes and verify through simulations that it is acceptable to ignore independence. However, at the moment, we have not found a way to plug in equations (2) and (3) into the distribution of the maximum of n i.i.d. Since we found that disorder has opposite effects on hard and soft graphs, we plan to investigate in the future how the heaviness of tail of the connection function changes the properties of soft graphs. The main purpose of this studied model is to provide a method for modelling Ca sparks, but it also has wider applications, such as modelling the propagation of disease in plants [20] and the construction of cellular networks [21]. Due to time and capacity constraints, the networks simulated in this study are small and are mainly learned with physical accuracy. In the future, we hope to better validate the results of this study by optimising the code and using HPC clusters to obtain larger simulations.

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Appendix

A Maximum of identically and independently distributed random variables

Suppose we have n identically and independently distributed random variables $X_1, X_2, \ldots, X_n$ with common probability mass function $f_X(x)$ and cumulative distribution function $F_X(x)$. To find the expectation and variance of $\text{Max}\{X_1, X_2, \ldots, X_n\}$, we first need to find it's distribution. Denote random variable $\text{Max}\{X_1, X_2, \ldots, X_n\}$ as M, then we have the following equation.

$$\begin{aligned} F_M(m) &= P(M \leq m) \\ &= P(Max\{X_1, X_2, \ldots, X_n\} \leq m) \\ &= P(\bigcap_{j=1}^{n} \{X_j \leq m\}) \\ &= \prod_{i=1}^{n} P(X_i \leq m) \end{aligned}$$

Since X is independent to each other

$$\prod_{i=1}^{n} P(X_i \leq m) = F(m)^n$$

To find p.d.f. of M, we differentiate above equation and obtain the following

$$f_M(m) = n f_x(m) F_x(m)^{n-1}, \tag{10}$$

This yields the mean and the variance of the maximum as

$$E(M) = \sum_{i=1}^{n} mn f_x(m) F_x(m)^{n-1}, \tag{11}$$

$$Var(M) = \sum_{i=1}^{n} m^2 n f_x(m) F_x(m)^{n-1} - E(M)^2. \tag{12}$$

B Code for python simulations

GitHub link source code of PLGG simulations:

https://github.com/AndyYueWu/Properties-of-PLGG