Physics-guided data-driven modeling to understand complex phenomena and to solve real-world problems

UROP1100 Progress Report

Cheng Chun Hei

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1 Abstract

Active matter and resistor networks are studied using a network science approach as these complex systems can be considered as networks. The Vicsek model of active matter is modified by adding smooth rotation of particles and decay of weight of links between particles with distance. The simulation results of these modifications are compared to examine their effects on the model. We also studied the change of voltages at each junction in a regular, hexagonal resistor network after removing resistors. This may allow us to train a machine learning model to detect broken resistors in a resistor network with the voltage changes from a few nodes.

2 Introduction

In this project, network science concepts are used to analyze complex physical systems including active matter and resistor networks. Network science is a field which studies complex systems by considering the elements in the systems as nodes and connections in the system as links to represent the systems as networks [1].

The Vicsek model is a simple and popular model of active matter. In this model, identical particles undergo random walk at constant speed and align their direction of motion to the average direction of their neighbors [2]. Many different modifications have been made to the model to make it more realistic. We modified the Vicsek model to introduce smooth rotation of particles and decay of weight of links between particles with distance in this project.

A network science approach is used to analyze different resistor networks. Junctions and resistors in a resistor network can be represented by nodes and links respectively. The weight of each link is proportional to the conductance of the corresponding resistor. By solving the voltage at the nodes in the network computationally, the effects of changes in the network structure on the voltages can be examined.

3 Methodology

The motion of particles in the original Vicsek model can be described by this set of three equations

$$\theta = \langle\theta\rangle_R + \eta\epsilon \tag{1}$$

$$\mathbf{v} = v_0 e^{i\theta} \tag{2}$$

$$\frac{d\mathbf{r}}{dt} = \mathbf{v} \tag{3}$$

where **r** is the position, **v** is the velocity, v_0 is the linear speed and θ is the direction of motion of the particle. In equ. (1), the $\langle\theta\rangle_R$ term is the mean direction of all particles within the distance R of the particle and the $\eta\epsilon$ term is an intrinsic noise added to the direction where η is the noise parameter and ϵ is a random number in range in the range $[-\pi, \pi)$. The behaviour of this simple model is controlled by only two parameters, the noise parameter η and the density of particles ρ [2].

In our modification of Vicsek model, the new equations of motion are

$$\frac{d\theta_i}{dt} = f\left(\text{Angle}[\sum_j^N w_{ij}\mathbf{v}_j] - \theta_i\right) + \eta\epsilon \tag{4}$$

$$\mathbf{v} = v_0 e^{i\theta} \tag{5}$$

$$\frac{d\mathbf{r}}{dt} = \mathbf{v} \tag{6}$$

$$w_{ij} = \begin{cases} \frac{1}{(1+d_{ij})^a},\ d_{ij} \leq R \\ 0,\ d_{ij} > R \end{cases} \tag{7}$$

. In equ. (4) the direction θ is updated with a rate of change proportional to a rotation parameter f and based on the difference between the direction of the particle and the weighted average direction of nearby particles instead of the instant change in the original Vicsek model. This system of particles can be viewed as a network in which each particle is a node and links are connected between each pair of nodes with distance $< R$ with weights as a function of the distance given by equ. (7). The weight w_{ij} in the weighted average direction is the element (i, j) the adjacency matrix of the network. The decay parameter a describes how quickly the influence of a particle affects other particles as the distance between them increases. This model returns to the original Vicsek model when $a = 0, f = \frac{1}{\Delta t}$.

An order parameter

$$\Phi = \frac{1}{N v_0} \left| \sum_{i}^{N} \mathbf{v}_i \right| \tag{8}$$

, where N is the number of particles and $\mathbf{v}_i$ is the velocity of the i-th particle, can be defined to describe how well the particles align with each other. The stationary order parameter Φ, which is average instantaneous order parameter when the system reaches an equilibrium, can be used to identify the phase of the system with $\Phi \approx 1$ being the coherently moving phase and $\Phi \approx 0$ being the completely disorganized phase.

In the simulation, particles are placed in a 2d square box with periodic boundaries at an initial density of $\rho = 0.5$. The simulation is run for 200 time steps and the last 20 time steps are used in the calculation of stationary order parameter Φ.

The second problem that we have studied is the effect of removing links in a resistor network. In the network science perspective, a resistor network can be represented by an adjacency matrix C with each element C_{ij} representing weight of the link between node i and j equal to the conductance of the resistor between the two nodes. By Ohm's Law, the current from node i to j is given by

$$I_{ij} = \frac{V_i - V_j}{R_{ij}} = (V_i - V_j)C_{ij} \tag{9}$$

where V_i is the voltage at node i. By Kirchhoff's rule, the sum of current flowing from a node i is

$$\sum_{j}^{N} I_{ij} = \sum_{j}^{N} (V_i - V_j)C_{ij} = 0 \tag{10}$$

. This can be written into matrix form $AV = \mathbf{0}$ with

$$A_{ij} = \begin{cases} -C_{ij},\ i \neq j \\ \sum_j^N C_{ij},\ i = j \end{cases} \tag{11}$$

. If a voltage source V_{in} is supplied to node i ($V_i = V_{in}$), Kirchhoff's rule no longer apply to that node so all elements in the i-th row of A is 0 except $A_{ii} = 1$ and the V_{in} is added to the i-th element of the vector on the right hand side. The resulting linear equation can be solved computationally to obtain the voltage V at each node. This allows us to examine the changes in voltage at each node of the network after link removals.

4 Results

At $a = 0, f = \frac{1}{\Delta t}$, our modification of the Vicsek model produces results similar to the original Vicsek model as shown in animation 1 (see appendix). In fig. (1) the stationary order parameter has a smooth transition from 1 at no noise to 0 at noise $\eta = 1$ as expected.

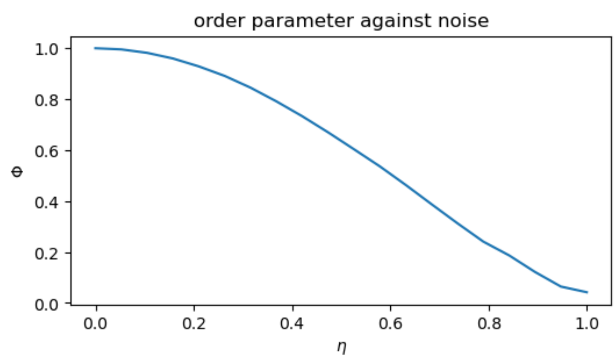


Figure 1: Stationary order parameter with $a = 0, f = \frac{1}{\Delta t}$

When $f < \frac{1}{\Delta t}$, each particle rotates slowly towards the average direction of their neighbours so they behave more disorderly at the same noise level as shown in animation 2. This is also shown in fig. (2) where the stationary order parameter decreases as f decreases.

At $a > 0$, the effect of the direction of a particle on their neighbour decreases as the distance between them. This decreases the effective range of neighbour detection of a particle as a increases since the effect of the neighbours further away decreases. Therefore, the stationary order parameter decreases as a increases as shown in fig. (3). There is also an unexpected clustering behaviour as shown in animation 3. We do not have a good interpretation of the phenomenon yet, but we

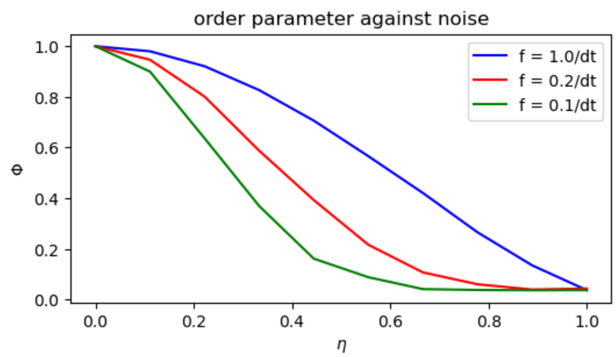


Figure 2: Stationary order parameter at different f with $a = 0$

hope to find a quantity to describe the clustering of particles so that we can analyze this more quantitatively and better understand the cause of this behaviour in the future.

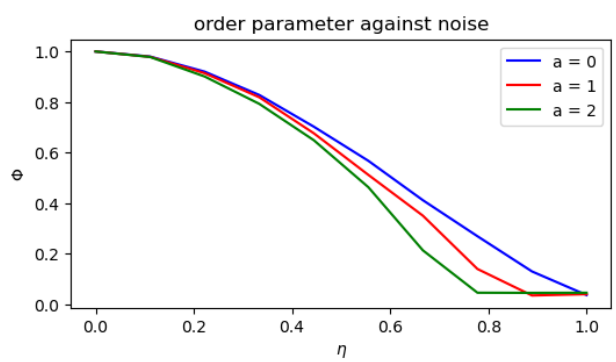
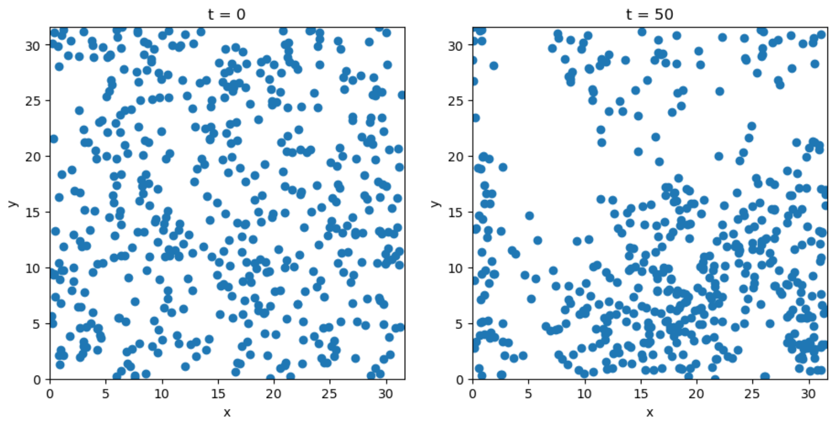


Figure 3: Stationary order parameter at different a with $f = \frac{1}{\Delta t}$

The regular hexagonal resistor network shown in fig. (5) with voltage input V_{in} at the center left node and ground at the center right node is examined in this project. This network chosen for its symmetry and visual clarity so that it be analysis more easily.

In fig. (6), the voltage change at each node when a link is removed is plotted.



(a) (b)

Figure 4: Snapshots of animation 3

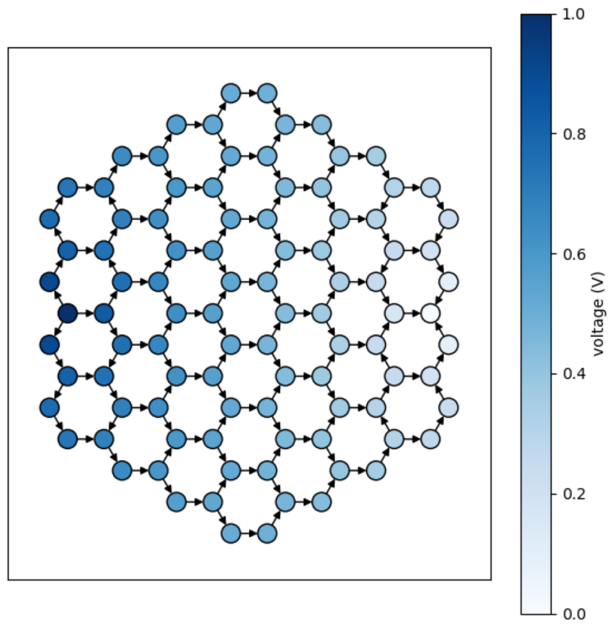


Figure 5: Voltage and current in hexagonal resistor network

A dipole-like pattern can be seen around the removed link with the side closer to the voltage input being positive and the side closer to the ground being negative.

Therefore, there is no simple relationship between the voltage change of a node and its Manhattan distance from the removed link.

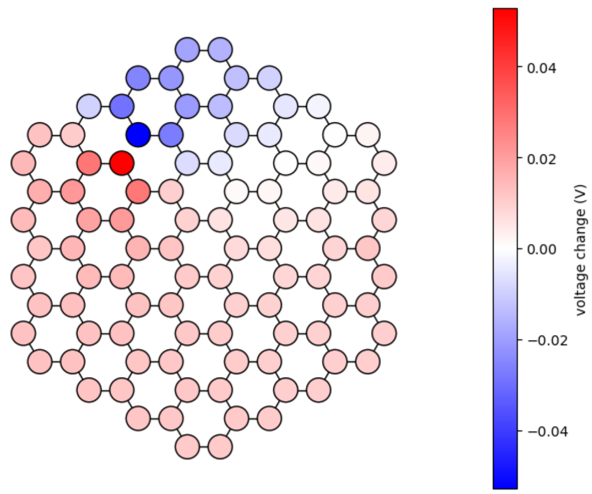


Figure 6: Voltage changes in hexagonal resistor network with one link removed

In fig. (7), the sum of the absolute voltage change at all nodes for each link removal is represented by the colour of the corresponding link. Only one link is removed at a time and the network is restored to its original state before another is removed. The removal of links closest to the voltage sources have the greatest impact on the network.

In fig. (8), the voltage change at a selected (green) node when each link is removed is plotted at the corresponding link. Generally, the removal of links between the selected node and voltage input tends to cause negative voltages changes at the node and the opposite happens between the selected node and the ground as expected. However, some outliers that do not follow this pattern can be seen in both figures. There are many factors which affect the voltage change of a node

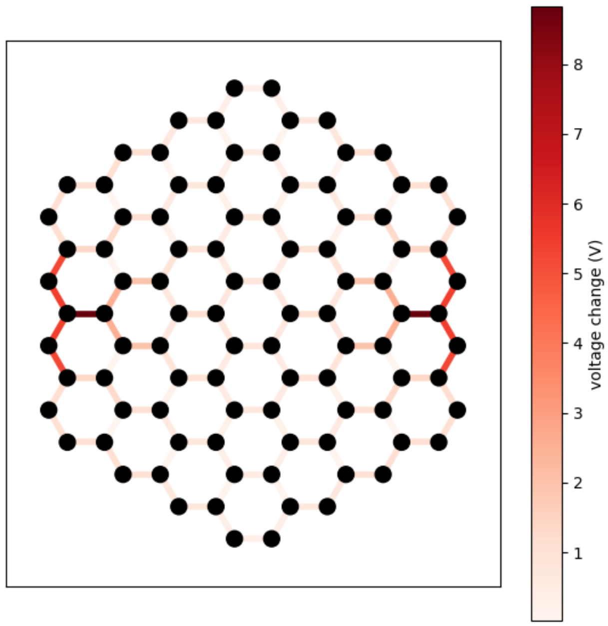
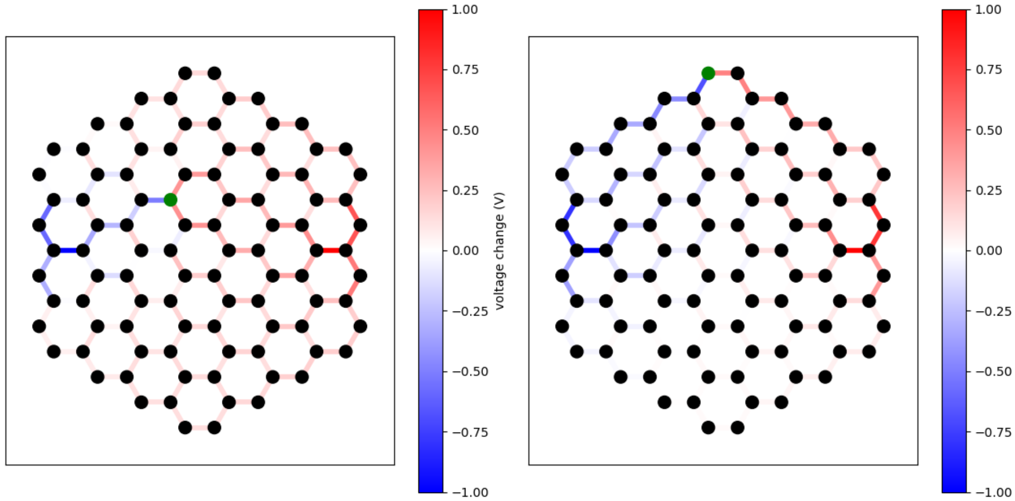


Figure 7: Sum of the absolute voltage changes with each link removed

when a link is removed, so it is very difficult to find a simple rule to identify the removal of a link from the voltage of a node. Since the sets of possible removed links given by the voltage changes at different nodes are different, it may be possible to find the removed link from the overlap between them using only a few nodes. Our future research direction is to use machine learning to identify the link removed by only detecting the voltage changes at a few different nodes.



(a) (b)

Figure 8: Voltage change of selected (green) node with each link removed

5 Conclusion

In this project, we studied modifications of the Vicsek model and the effect of link removal in resistor networks. From simulations, we observed that particles in the Vicsek model behave more disorderly when they rotate more slowly and their weights decay more rapidly. We plan to further study the clustering behaviour of particles with decaying weights in the future. The voltage changes after link removal in a resistor shows a dipole-like pattern around the removed link. Our future direction is to gain a better understanding on the effect of link removal on different nodes to train a machine learning model to detect broken resistors in a resistor network.

6 Appendix

Animation 1: Vicsek model with $a = 0,\ f = \frac{1}{\Delta t},\ \eta = 0.3$

https://drive.google.com/file/d/1rCee_YqODCdNHRmN60UoTKX-j2BK7lYO/view?usp=sharing

Animation 2: Vicsek model with $a = 0,\ f = \frac{1}{5\Delta t},\ \eta = 0.3$

https://drive.google.com/file/d/1vVeZ7z18lZ5BO70exy6wAirQEFSQHyEX/view?usp=sharing

Animation 3: Vicsek model with $a = 1,\ f = \frac{1}{\Delta t},\ \eta = 0.3$

https://drive.google.com/file/d/1aIl6q2KKUkDR_tB8MY0mlw1QW_E9PFky/view?usp=sharing

References

[1] Barabási, A.-L. Network science. *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences 371*, 1987 (2013), 20120375.

[2] Vicsek, T., Czirók, A., Ben-Jacob, E., Cohen, I., and Shochet, O. Novel type of phase transition in a system of self-driven particles. *Physical Review Letters 75*, 6 (aug 1995), 1226–1229.