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Visual Analytics of Global Parameters in Simulation Ensembles of ODE-based Excitable Network Dynamics

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Abstract

The role of network topology on the dynamics in simulations that are executed on the network is a central question in the field of network science. However, the influence of the topology is affected by the global dynamical simulation parameters. To investigate this impact of the parameter settings, multiple simulation runs are executed with different settings. Moreover, since the outcome of a single simulation run also depends on the randomly chosen start configurations, multiple runs with the same settings are carried out, as well. We present a visual approach to analyze the role of topology in such an ensemble of simulation ensembles. We use the dynamics of an excitable network implemented in the form of a coupled ordinary differential equation (ODE) following the FitzHugh-Nagumo (FHN) model and modular network topologies.

1 Introduction

How topological structures of networks influence the dynamical processes simulated on the networks has been a core question for neuronal scientists and computational biology experts in recent years [MHKH15, PS15, RRGS12, KLP*17, BSS15, NHL16]. Many dynamical models, which can be either discrete [NHL16] or continuous [MHKH15], have been studied to elucidate the relationship between connectivity structures and functional structures of networks. In those models, parameter settings can determine in which regimes the dynamics are influenced by topology of the networks [KP03]. One of the most famous models that has been investigated in that regard in computational neuroscience is the FitzHugh-Nagumo model (FHN), which simulates neural dynamics [MHKH15]. Depending on the parameter settings, the dynamics of the network can be operated in three different regimes, namely excitable, oscillatory, and bistable [KP03].

Besides those parameters which decide what regime the dynamics follow, there are other parameters confirmed to be deciding factors on the outcome of the dynamics within a regime [HJBS06]. The effect of those parameters on spatiotemporal patterns on discrete models has been intensively studied recently [MLHH08, NHL16, MLMH06]. In particular, the network activity patterns at the global scale of the networks, such as the synchronization of nodes within a module in their co-activation patterns or the co-activation waves around hubs, have been examined at different levels of spontaneous parameters in a discrete dynamical model [MLHH08, NHL16]. Similar studies have been conducted with continuous dynamical models, but only at a local, not at a global scale of the underlying network. For example, one study investigated the noise effect on the co-activation pattern of the FHN model for a network of only two nodes [HJBS06]. To our knowledge, the effect of the parameters such as noise at a global scale has not been addressed yet for continuous models. We present a visual analytics approach in analyzing simulation ensembles to fill this gap. Using the noise parameter as an example, the effect of such parameters on the role of topology for the dynamical patterns at a global scale is studied systematically in an excitable regime of the continuous ODE-based FHN model. Our approach is based on using multiple coordinated views with multi-dimensional scaling (MDS) plots for showing dynamical behavior within an ensemble of simulations and a network visualization for showing the topology. The dynamical and topological views are linked via interaction mechanisms to allow for analytical reasoning.

2 Simulation Model

Given an undirected network (or graph), let D denote its adjacency matrix. Then, the FHN dynamics operating on the network is described in the form of an ODE of two nested variables, in which variable x is called the membrane potential and y the recovery variable [MHKH15]:

$$\begin{cases} \tau_x \frac{\partial x(t)}{\partial t} & = & \gamma x(t) - \frac{x^3(t)}{3} - y(t) + kDx(t) + \sigma v_x(t), \\ \tau_y \frac{\partial y(t)}{\partial t} & = & \beta y(t) + x(t) + \alpha + \sigma v_y(t). \end{cases}$$

Setting the global parameters $\alpha = 0.909, \beta = -0.391$, and $\gamma = 1.688$ we perform simulations in an excitable regime. The time scale parameters τ_x, τ_y, and the global coupling strength k, are accordingly set to 1.0, 100.0, and 0.025, respectively. Moreover, $v(t)$ stands for an uncorrelated Gaussian noise with zero mean and unit

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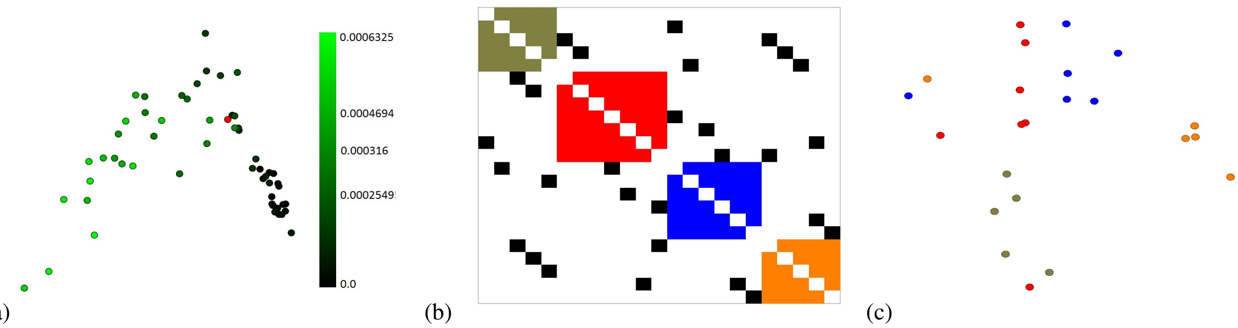

(a) (b) (c)

Figure 1: *(a) The MDS projection of multiple noise intensity settings, the color encodes the value of noise intensity; the red point indicates a selection. (b) The adjacency matrix visualization of the network with different colors for different modules. (c) The MDS projection of dynamics in the noise intensity selected in (a); the color encodes which modules the corresponding nodes belong to in the network in (b).*

variance whose amplitude is scaled by σ. To investigate the impact of the noise parameter, multiple simulation runs are executed with different values for σ in the range from 0 (no noise) to 0.0006325. Moreover, since the outcome of a single simulation run also depends on the randomly chosen start configurations, multiple runs with the same noise settings have to be carried out, as well. After performing all simulations, for each noise setting we have an ensemble including time series of all nodes in the network for each simulation run. Hence, the overall output can be described as an ensemble (with different noise settings) of ensembles (with same noise settings, but different random initial conditions). The topology of the network remains the same for all simulation runs. We are using a modular network with four modules as shown by the different colors in the adjacency matrix in Figure 1(b).

3 Similarity Within and Between Ensembles

To measure similarity of nodes within one simulation run, we detect spikes of activation in the time series and compute the co-activation matrix [MHKH15], which encodes how frequently two nodes have simultaneous excitation. For each ensemble of runs with the same noise setting, we compute the average co-activation matrix of all those runs. The resulting matrix provides the characteristic property to evaluate how much dynamics are influenced by the topological structures of the network. To compare two ensembles of different noise settings, we interpret the respective average co-activation matrices as vectors and compute their correlation. This can be done pairwise for the ensembles of all the different noise settings leading to a correlation matrix, which captures the pairwise similarities between all ensembles.

4 Visual Encoding and Interactive Analysis

To evaluate the influence of the network topology on the dynamics for one noise setting, we use a topological and a coordinated dynamical view [NHL16]. The *dynamical view* is generated by computing an MDS layout on the co-activation matrix. Distances in the plot encode the similarity between the time series of the nodes (rendered as points). For an ensemble of one noise setting, we use the average co-activation matrix, see Figure 1(c). The *topological view* shall encode the modular structure, which is best done using the adjacency matrix, see Figure 1(b). To visualize the similarity between ensembles of different noise settings, we compute an MDS layout on the correlation matrix described above. Here, distances encode similarities between ensembles, which are shown as points with color encoding the value of the noise parameter. This *ensemble view* is shown in Figure 1(a).

The three views are coordinated allowing for selection in one and highlighting in other views. Figure 1 shows how one ensemble (red dot) is selected in the *ensemble view* (a) and shown in the other views. In the *topological view* (b), the four modules were selected and highlighted by color. The same colors are used in the *dynamical view* (c) to investigate whether the topological groups also form dynamical groups.

5 Results

When examining the *ensemble view* in Figure 1(a), the lowest noise levels (≤ 0.0002) form a cluster (dark points on the right). Examining them in the *dynamical view* with the selections shown in the *topological view* (b) revealed that topology has no effect, as basically the time series of all nodes synchronize. For medium-sized noise levels (between 0.0002 and 0.0004694), the *ensemble view* (a) also exhibits a cluster (upper medium-bright points) and the *dynamical view* (c) reveals a clear matching of topological and dynamical similarity, i.e., topology drives the dynamics. For large noise levels (≥ 0.0004694), the dynamical behavior becomes random, which can be observed by the ensembles forming again a cluster (bright points on the lower left) in the *ensemble view* (a), while the *dynamical view* shows no matching with the topology.

6 Conclusions

We have presented a visual analytics approach to evaluate the effect of noise on the influence of topological structures for excitable network dynamics. We have observed that there are three groups of ensembles and were able to interpret the result using coordinated views.

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