Vision, Modeling, and Visualization (2019)
H.-J. Schulz, M. Teschner, and M. Wimmer (Eds.)

Visual Analytics of Simulation Ensembles for Network Dynamics

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Abstract

A central question in the field of Network Science is to analyze the role of a given network topology on the dynamical behavior captured by time-varying simulations executed on the network. These dynamical systems are also influenced by global simulation parameters. We present a visual analytics approach that supports the investigation of the impact of the parameter settings, i.e., how parameter choices change the role of network topology on the simulations' dynamics. To answer this question, we are analyzing ensembles of simulation runs with different parameter settings executed on a given network topology. We relate the nodes' topological structures to their dynamical similarity in a 2D plot based on an interactively defined hierarchy of topological properties and a 1D embedding for the dynamical similarity. We evaluate interactively defined topological groups with respect to matching dynamical behavior, which we visually encode as graphs of the function of the considered simulation parameter. Interactive filtering and coordinated views allow for a detailed analysis of the parameter space with respect to topology-dynamics relations. Our visual analytics approach is applied to scenarios for excitable dynamics on synthetic and real brain connectome networks.

1. Introduction

Network Science is "the study of network representations of physical, biological, and social phenomena leading to predictive models of these phenomena" [Cou05]. A core research question is how topological structures of networks influence dynamical processes that operate on the networks [MHKH15,PS15]. A prominent example of network dynamics are excitable dynamics [MLHH08,HL09] that play an important role in many biological processes such as brain activity [SCKH04].

When running dynamical simulations on network structures, the dynamics typically depend on a number of global model parameters. The choice of these parameters affects the dynamics and, consequently, may also change the effect of topology on the dynamics. Such investigations have been conducted by observing the correlation between topological and dynamical matrices, where the topological matrices are computed to reflect the topological structures of either modules or hubs, while the dynamical matrices reflect the dynamical similarities of the network's nodes [HL09, MLHH08]. Such analyses reside on the level of a few specific observations. A more exhaustive investigation requires a systematic approach on entire simulation ensembles.

We work towards closing this research gap by proposing a visual analytics approach for analyzing the influence of global simulation parameters on the role of network topology for the dynamical behavior. Our approach takes as input an ensemble of simulation runs that have been executed with various global parameter settings on a given network, see Section 2. To relate topology to dynamics, we propose to use a 2D plot that embeds dynamical similarities of the networks' nodes and relates them to interactively detected topological features, see Section 3. Furthermore, we propose a parameter space visualization that illustrates the matching of selected topological groups with their dynamical behavior as graphs of a function over the investigated simulation parameter. Interactive filtering operations and coordinated interaction among the proposed views allow for an intuitive and effective analysis of the entire ensemble at different levels of aggregation. The proposed methodology is a combination of interactive visual analysis steps with automatic data mining/statistical computations. The analytical workflow consists of selecting topological structures, followed by analyzing their relation to dynamics, and eventually of parameter space investigations, which allow for analytical reasoning on which parameter settings reflect which behavior. We apply our methods for the analysis of excitable network dynamics simulation ensembles on synthetic networks and cortical connectivity networks of the cat brain. We report our findings in Section 4. Our main contributions can be summarized as:

- A novel visual analytics approach to analyze the influence of global parameters on the role of network topology for the dynamical behavior in excitable network dynamics.
- A user-centric network topology analysis to define potentially relevant topological structures for relating them to dynamics in further analysis steps.
- A 2D plot for relating topological structures to dynamical node similarities.
- A parameter-space visualization that reveals topology-dynamics

DOI: 10.2312/vmv.20191322

matches at an overview level and allows for coordinated interaction with more detailed views.
- Application to synthetic and real-world data for novel findings.

2. Background and related work

Simulating dynamics on networks requires the scientist to choose a network architecture that is to be investigated and a dynamical model that is to be executed on the network. Varying the global parameters of the dynamical model leads to a network dynamics simulation ensemble. In the following, we will provide the necessary background of such simulation processes.

Network architecture. A network is an abstract concept representing the connectivity between entities, to which we refer to as its topology. A network is represented by an undirected graph.

Topological structures. The network topology may exhibit certain structures or features. Two universal patterns in the topology of networks are modular structures, which are common in biological networks such as the human brain connectome [PS15, MLHH08], and central nodes (referred to as hubs) [MLHH08]. A subset of nodes are said to form a *module*, if there exists a denser level of connectivity among them than connections to nodes outside of the subset. Hierarchical modular structures refer to nested levels of connectivity, i.e., a modular structure can be (iteratively) decomposed into denser submodular structures. It is ongoing research in biology to study the role of hierarchical modular structures in networks such as the human brain connectome [KH10, PS15, MLHH08]. The degree of a node is defined as its number of edges. A *hub* is a node with dominant degree, i.e., its degree is larger than those of other nodes of the network. Using the tool we present in this paper, the user may define and investigate any topological structure, but due to the general interest in modules and hubs, we focus on such structures in the application scenarios.

Network examples. Network architectures that we are going to investigate include a hierarchical modular network with 60 nodes [KH10], which we generate using a hierarchical modular network model [PS08], see Figure 1, and a hierarchical network with 256 nodes [RSM*02, HL09] containing modules and hubs, which we generate using the iterative scheme described in [RSM*02], see Figure 5. Moreover, we investigate the cat brain connectome network with 55 cortical and subcortical regions obtained by tract tracing [SCKH04, HK04], see Figure 8. It describes system-level connections between different areas of the cat cerebral cortex, is based on a global collation of cat cortical connectivity (892 interconnections of 55 areas) [SBY95], and is part of a larger database of thalamo-cortical connectivity of the cat [SBH*99], which was created by the interpretation of a large number of anatomical reports of tract-tracing experiments. It is an almost symmetric directed network that is commonly transformed to an undirected network for analyses [BS09].

Dynamical model. Many dynamical models have been studied to elucidate the relationship between connectivity structures and functional structures of networks. The outcome of a dynamics simulation run is a time series for each node of a given network, where the values of the time series change according to the chosen dynamical model operating on the given network. Since the real-world examples in our application scenarios are brain networks, we focus – as a proof of concept – on excitable network dynamics that are commonly used to simulate brain activity [SCKH04]. A simple and parameter-sparse implementation of such dynamics is a discrete stochastic cellular automaton, which is referred to as the 'susceptible, excited, recovering' (SER) model and has been extensively investigated to simulate excitable neural dynamics, e.g., [MHKH15, MLHH08, NHL16]. To each node one of the three states excited (E), recovering (R), or susceptible (S) is assigned. In each simulated time step, a node in state R turns into state S with a probability p, which is called the recovery rate (or otherwise stays in state R). A node in state S turns into state E, if at least one neighbor node is excited. Even if no neighbor node is excited, a susceptible node may turn spontaneously into state E with a probability f, which is called spontaneous ignition rate. Finally, a node in state E always turns into state S in the next time step.

Simulation ensemble. The parameters p and f introduced above are global parameters that affect the overall dynamical behavior. The user may use our system to select the range in parameter space and its sampling to generate an ensemble. To demonstrate how our visual analytics approach supports analyzing the effect of these parameters, we analyze ensembles with varying values of f (while keeping $p = 0.1$ fix) and between $1,000$ and $8,000$ simulation runs.

Dynamical similarity. In order to investigate, which topological structures affect the dynamical behavior, we need to analyze, how information propagates through the network. Thus, we need to identify, which nodes of the network have a similar dynamical behavior, i.e., we need to define a similarity (or distance) measure for the time series generated per node. The similarity measure can be computed pairwise, i.e., for each pair of nodes in the network. The pairwise similarities can be stored in a symmetric similarity matrix. How the similarity is computed, depends on the dynamics that are simulated. For excitable dynamics, one typically captures similarity by a co-activation measure, which calculates how often a pair of nodes is simultaneously active (excited) [MLHH08, NHL16]. For the SER model, the co-activation coefficient between two nodes is computed by

$$C_{ij} = \frac{1}{N} \sum_{k=0}^{N-1} \delta(T_k^i, T_k^j) \tag{1}$$

where N is the number of time steps, T_k^i the state of node i at time step k, and $\delta(T_k^i, T_k^j) = 1$ if $T_k^i = T_k^j = E$ and 0 otherwise. The matrix C whose elements are the co-activation coefficients is called the co-activation matrix. For each simulation run, i.e., each parameter setting, we can compute one co-activation matrix.

Network visualization. The most common network visualization approaches use node-link diagrams based on a wide range of layout algorithms such as the force-based one used in Figure 5(a), adjacency matrices as in Figure 5(b), or combinations thereof. Node-link diagrams suffer from visual clutter when networks become large and dense. Although the sizes of the networks in our application scenarios rarely exceed tens or hundreds of nodes, they may be dense and the node-link diagrams may exhibit clutter, cf. Figure 5(a). The topological structures are better recognized in adjacency matrix visualizations as long as a suitable order is established [BBHR*16]. Thus, an adjacency matrix visualization is one

of the main interactive views we are using to discover and select modular structures of the network. To detect and select hubs, Ngo et al. [NHL16] proposed a treemap layout, where size corresponds to the nodes' degrees. Their space-filling approach is compact, but barcharts, generally, allow for better quantitative comparisons of the sizes, which is why we chose them for hub selection.

Visualizing dynamical processes on networks. Early attempts for visualizing dynamical processes on networks plotted time series in conjunction with topological structures [JKS06]. Such time-series visualization of individual nodes cannot reveal global topological structures that govern the dynamics. Ngo et al. [NHL16] introduced a visual analytics approach to discover how topological structures such as hubs, modules, or hierarchies in networks influence the dynamical processes. However, they only looked at individual simulation runs and not at simulation ensembles.

Ensemble analysis. In network dynamics models, there are parameters confirmed to be decisive factors on which outcome to be expected [HJBS06]. The effect of those parameters in spatio-temporal patterns has been intensively studied using purely analytical approaches [MLHH08, HL09]. These studies typically focus on some selected parameter settings and some selected topological structures. Our user-centric approach instead analyzes entire ensembles of densely sampled parameter spaces to analyze how patterns emerge as a function of the parameter settings. Moreover, it allows for the interactive detection, selection, and exchanging of multiple topological structures that are to be investigated.

Visualization of simulation ensembles has gained increasing attention over the last decade [WHLS19]. A conceptual framework for visual parameter-space analysis was presented by Sedlmair et al. [SHB*14]. Using their notation, we follow a global-to-local strategy, where the task is related to parameter-space partitioning. Like us, Luboschik et al. [LRB*15] studied the influence of parameters on dynamical systems, but their dynamics are not defined over networks and their task is, therefore, much different from ours.

3. Methodology

3.1. Design goals, space, and choices

There are three facets in our data that we want to relate to each other. First, there is the topology of the network that is considered to be static. Second, there are the dynamics that are simulated on the network and we would like to relate the dynamics to the topology. Third, there are global parameters that change the overall dynamical behavior when being adjusted.

Since our goal is to determine which topological structures are mainly responsible for the propagation of excitation in the dynamics, we want to capture both topological similarity between nodes of a network as well as their dynamical similarity. Following examples from literature (see above) one may compute a topological and a dynamical similarity matrix for the nodes and try to relate them to each other. However, this would require us to know, what topological structures we should consider, which is what we are actually trying to find out. Hence, we want to formulate the first design goal that we need to have a flexible interactive analysis component for the network topology that allows us to quickly and intuitively define topological structures for further investigation. Moreover, since multiple topological structures may compete and different conclusions may be drawn for different parameter settings, we want to be able to define multiple topological structures simultaneously for a joint analysis. We present a respective topological analysis for defining possibly relevant topological structures in Section 3.2.

Our second design goal is to relate the defined topological structures to dynamical behavior. An obvious choice would be to use coordinated views of topological structures and dynamical behavior to interactively analyze their commonalities using filtering, selection, and highlighting mechanisms. However, since we may need to analyze this relationship for many simulation runs, an excessive interactive sessions should be avoided. Instead, a simple 2D view that integrates both topological and dynamical aspects would be desirable. We propose a simple scatterplot-like visualization for relating topology to dynamics, see Section 3.3.

Finally, we want to investigate an entire ensemble of simulation runs with varying parameter settings. Hence, our third design goal is a parameter-space visualization that provides an overview in the form of aggregated topology-dynamics matching for all simulated parameter settings. We compute respective matchings of all selected topological structures to the simulated dynamics and display them as a graph of a function over the investigated parameter, see Section 3.4.

3.2. Topology analysis

In the topology analysis, one wants to explore the existence of certain topological structures using respective visual encodings and layouts and to have means for interactive selections of observed structures. Moreover, one wants the system to support automatic extraction of groups that are formed by certain topological properties. Since different structures are best conveyed in different visual encodings, we propose to use two visual encodings that allow for the interactive definition of potentially interesting structures.

Arguably the most commonly used visual encoding of network topology is a *node-link diagram*, where node positions are determined by a range of different layout methods. As discussed above, such node-link diagrams can quickly lead to visual clutter when the networks are not sparse, cf. Figure 5(a). Although our implementation supports node-link diagrams with a force-based layout, we do not recommend to use them, unless networks are sparse.

Another common visual encoding of network topology are *adjacency matrices*. When using a suitable ordering such as the barycenter ordering [McG12], an adjacency matrix supports the detection of modules. They can also be easily selected within the visual representation. Figures 1(a),(b) show an example where the adjacency matrix reveals some modular structures. The individual modules are selected and each module is assigned to a topological group and labeled accordingly with user-defined colors chosen from a color picker. If the modules form a dominant topological structure for the dynamics, one would expect the dynamics of each module's nodes to synchronize, i.e., the time series of all nodes within the selected topological structures would assimilate over time.

Hubs are also visible in adjacency matrix layouts, but the exact degree and sorting of multiple hubs within a network is not so

easily recognizable. The degrees of nodes can be most easily quantified and compared using barcharts with decreasing order, see Figure 5(c). When a hub is selected, layers around the hub (i.e., groups of nodes with same distance to the hub) are automatically generated to form topological groups. If the hub forms a dominant topological structure for the dynamics, one would expect the dynamics of the nodes in each layer to synchronize.

3.3. Relating topology to dynamics

Having defined the topological groups that are to be investigated, we want to relate them to the dynamics. We propose an integrated view of both aspects that exhibits the relation using an intuitive 2D scatterplot-like encoding, where each point corresponds to one node for a selected simulation run. To position the nodes in the plot, the vertical axis shall reflect dynamical similarity, while the horizontal axis shall reflect topological groupings.

The *vertical axis* is defined by a 1D embedding of the dynamical similarity. Starting with the co-activation matrix defined in Equation 1, we normalize the values to the range $[0,1]$ and take one minus the normalized values to compute a distance matrix. This distance matrix can be fed to a dimensionality reduction method to compute the 1D embedding. Multi-dimensional scaling (MDS) and its variants are common strategies to generate such embeddings trying to preserve distances. Various distance measure calculations exist, leading to the different variants. Recently, the t-stochastic neighborhood embedding (t-SNE) algorithm [vdMH08] has proven to be very effective in a range of applications, where groups of similar data points shall be preserved. Since our goal is to observe groups of nodes that have similar dynamics, t-SNE is a suitable approach for our purposes.

Since we plan to investigate the dynamical similarities over varying parameter settings for the dynamical simulation ensemble, we would like to have a coherence of the embeddings for similar parameter settings. Since the embeddings depend on the initializations, such coherence cannot be assured when computing an embedding for each parameter setting independently. Instead, we adopt the dynamic t-SNE concept by [RFaT16]. Dynamic t-SNE modifies the t-SNE cost function by adding a terms that penalizes movement of points from one layout to the next. While the dynamical t-SNE approach tries to generate embeddings that vary smoothly over time, we use the dynamical t-SNE algorithm to create embeddings that vary smoothly over a given parameter. Thus, when using the dynamical t-SNE algorithm, a user may select not only a single simulation run, but also a range of parameter settings in the form of an interval of parameter values. Then, the points should stay at similar heights in the 1D embedding, if the outcomes of the simulation runs within the selected parameter interval do not vary much. To generate the embeddings, we follow the guidelines in literature to appropriately set the parameters [vdMH08,RFaT16]. Assuming the distance matrix to be of size $N \times N$, the t-SNE perplexity parameter ρ is chosen such that $3 \cdot \rho < N$. For dynamic t-SNE, the trade-off hyper-parameter is set to be $\lambda = 1.5$, the learning rate to $\eta = 250$, and the momentum coefficient to $\mu = 0.5$, where the momentum rate is changed from iteration 250 on and the maximum number of iterations for each optimization step is $1,000$.

The *horizontal axis* shall reflect the similarities with respect to the selected topological structures. Each selected topological structure defines groups (e.g., modules, submodules, or layers around one or multiple hubs). The nodes are then sorted along the horizontal axis to represent the groups. The groups are further visually encoded by drawing horizontal bars below the axis that are colored according to the colors chosen by the user when defining the topological structures. Since we are typically interested in analyzing multiple topological structures, the user can prioritize them. The first topological structure is then used to build the main groups for sorting the nodes. Within each group of the first topological structure the nodes are sorted with respect to the second topological structure, and so on. The prioritization of the topological structures forms a hierarchy, which we visually encode by cascading colored bars below the horizontal axis. The cascaded bars visualize the hierarchy similar to a bottom-up Icicle plot or a non-radial Sunburst diagram [SHS11]. The user may interactively change the prioritization by simple drag-and-drop operations on the rows of the cascaded layout, see Figure 7.

Given the 1D embedding of the dynamical similarity and the Sunburst layout of the topological groupings, the relations can be investigated. If the heights of all nodes of one topological group are equal or very similar, then the dynamics of the topological group seems to have synchronized. If the heights within a topological group are similar and, in addition, dissimilar to heights of nodes not part of the topological group, then one may deduce that the topological feature that was used to define the topological group directly impacts the dynamics. Following this rationale, one can interactively analyze different topological groups and their interplay.

3.4. Parameter-space visualization

For a large ensemble, it may be rather cumbersome to go through all simulation runs to detect matches of topological groups with dynamical behavior. Thus, we want to provide some guidance that allows the user to decide which parts of the parameter space may be interesting to investigate. We propose a parameter-space visualization, where the topology-dynamics matching is visualized over the entire range of the investigated parameter at an aggregated overview level.

As explained above, a topological group matches well the dynamics, if the co-activation of the nodes within the group is high and the co-activation of nodes inside the group to nodes outside the group is low. This formulation is close to the investigations made when trying to quantify the quality of a cluster. Hence, we can use concepts from judging clustering quality for our purposes.

A well-known measure for evaluating the quality of a cluster is the silhouette coefficient [Rou87]. We can adopt this measure to compute our topology-dynamics matching for each topological group. Let M be the topological group. Then, we can compute the average of the co-activation distances d_{ij} from a node $p_i \in M$ to any other node $p_j \in M$ by

$$a_i = \frac{1}{|M|-1} \sum_{p_j \in M, i \neq j} d_{ij} \; .$$

Following the idea of the silhouette coefficient, we can also compute the average co-activation distance from node $p_i \in M$ to nodes

$p_j \in N$, where N is the closest group to M by

$$b_i = \frac{1}{|N|-1} \sum_{p_j \in N, i \neq j} d_{ij} \; .$$

The silhouette equivalent for node p_i is defined by

$$s(p_i) = \begin{cases} 1 - \frac{a(i)}{b(i)} & \text{if } a(i) < b(i) \\ 0 & \text{if } a(i) = b(i) \\ \frac{b(i)}{a(i)} - 1 & \text{if } a(i) > b(i) \end{cases} \; .$$

The silhouette equivalent for the entire topological group M is then given as the average of the silhouette measures of all its nodes, i.e.,

$$s(M) = \frac{1}{|M|} \sum_{p_i \in M} s(p_i) \; .$$

With the given measure, we can judge the match of topological group M to the dynamics of each simulation run. The resulting values can be plotted over the parameter that has been varied when generating the ensemble. Thus, we get a parameter-space visualization in the form of a graph of a function that represents the matching quality of group M over changing parameter values. The user can interactively select which topological structures shall be examined. The respective graphs can be plotted in one diagram, which allows for a direct comparison of the matching quality of different topological structures. Figure 6 shows such a parameter-space visualization: eight topological groups are defined and the respective graphs of the matching quality are displayed over the parameter space. The colors of the graphs relate them to the topological groups defined in Figure 5.

3.5. Analytical workflow

The analytical workflow of a user when applying the methods, visual encodings, and interaction mechanisms outlined above for the analysis of excitable network dynamics simulation ensembles may be put into an iterative three-step process. The interactions made during a session are best documented in the accompanying video.

The first step is to analyze topological structures using the adjacency matrix and the degree barchart and to define which topological structures shall be analyzed. Our designs aim at selecting modules or hubs, but the user is free to define any group of nodes as a topological structure.

In the second step, the dynamics of the entire ensemble shall be matched against the topological groups defined in the first step. The user would investigate the ensemble as a whole by analyzing the parameter-space visualizations. The selected topological structures are fed to the Icicle layout, where the user can adjust the priorities to his/her liking and select groups for the display of its graph in the parameter-space visualization.

In the third step, the user would select individual simulation runs or parameter ranges from the parameter-space visualization based on the properties of the silhouette plots. The selection is performed by a simple horizontal slider within the parameter-space visualization. The selected simulation runs are then shown in the scatterplot that relates the topology to dynamics for the selected parameter settings. The horizontal slider allows for an intuitive traversal of the parameter space, while observing how patterns form or vanish in the scatterplots.

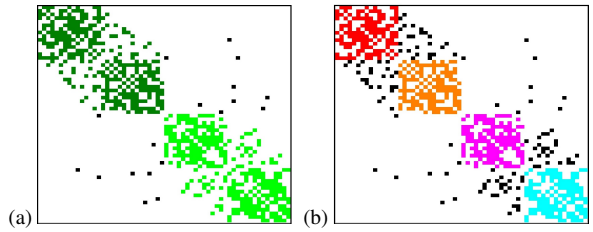

Figure 1: *Adjacency matrix of hierarchical modular network: Selection of modules (a) and sub-modules (b).*

Based on the insight obtained during this interactive visual analysis, the user may want to refine certain structures or iterate the process after re-ordering the attributes in the Icicle plot.

4. Results

We applied our methods proposed in Section 3 to the network architectures and simulation ensembles detailed in Section 2. The performed interaction operations are best observed in the accompanying video. The analytical workflow and analyses were discussed with a domain expert in the field of Network Science with application in Systems Biology, who was involved in the project from the beginning.

4.1. Synchronization in hierarchical modular networks

First, we are analyzing the hierarchical modular network shown in Figure 1. We can immediately see from the adjacency matrix that two large modules exist that split further into two submodules each. Hence, there are in total six modules at two levels. The figure shows their selection and color assignment. The Icicle plot is built according to these selections as in Figure 4. The modules can be selected to generate the parameter-space visualization, see Figure 2. The Silhouette curves are computed independently for each level, which satisfies the condition that clusters need to be disjoint for their computation.

When investigating the parameter-space visualization in Figure 2, we observe that all curves have a similar shape, i.e., they seem to be monotonically decreasing with a decreasing slope. However, the curves of the first-level modules are almost always lower than second-level ones. Thus, the sub-modules exhibit a slightly stronger influence on the synchronization pattern. However, for small values of parameter f, the Silhouette curves of first-level modules seem to be slightly larger. To observe that in more detail, we zoom into the range of low values. For a proper sampling, we computed further simulation runs in that range. Figure 3 exhibits that the curves are actually not monotonically decreasing, but first increase before they start decreasing. Moreover, it becomes apparent that the curves of the first-level modules are indeed higher than those of the second level. Thus, for small values of f, it is actually the first-level modules that exhibit a stronger influence on the synchronization pattern.

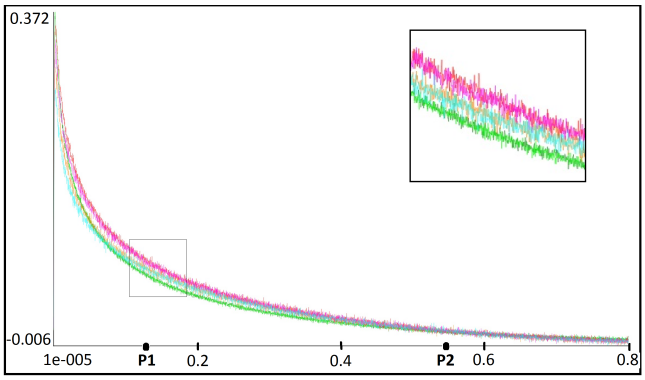

Figure 2: *Parameter-space visualization for parameter* $f \in [0.00001, 0.8]$ *with sample rate* 0.0001 *for topological structures selected in Figure 1. Silhouette curves are similar, but those of first-level modules are mostly slightly lower (see zoomed-in inset in the upper right).* $P1$ *marks interval* $[0.117274, 0.117496]$ *and* $P2$ *interval* $[0.549701, 0.549923]$ *for further investigation.*

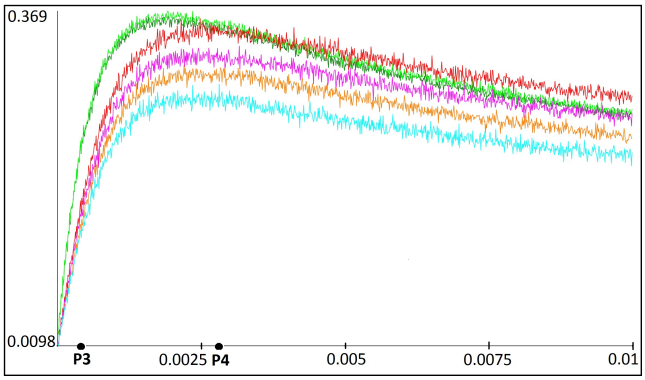

Figure 3: *Parameter-space visualization for parameter* $f \in [0.00001, 0.01]$ *with sample rate* 0.00001 *for topological structures selected in Figure 1. Silhouette curves are similar, but those of first-level modules are mostly slightly higher.* $P3$ *marks interval* $[0.00036625, 0.00037735]$ *and* $P4$ *interval* $[0.00271, 0.0027211]$ *for further investigation.*

We validate this observation using the 2D dynamics-topology plots in Figure 4 for intervals P1-P4 selected in Figures 2 and 3. P3 selects smallest values $f \in [0.00036625, 0.00037735]$. As expected, we see that the points assemble roughly at two heights matching the two first-level module structure, i.e., the nodes of the modules synchronize (Figure 4(a)). For slightly larger values of $f \in [0.00271, 0.0027211]$ selected by P4, the influence of the second-level modules is stronger, such that the points arrange themselves at roughly four heights matching the submodules (Figure 4(b)). This holds true for quite a large range of values for f, for example, it is still true for selection P1 with $f \in [0.117274, 0.117496]$ (Figure 4(c)). Finally, for large values of $f \in [0.549701, 0.549923]$ as in selection P2, the Silhouette values are low, i.e., the modules should not form visible structures anymore. This is confirmed by the 2D plot, where the point heights are rather random (Figure 4(d)).

4.2. Interplay of hubs and modules

In the second scenario, we analyze a network containing hubs and modules, see Figure 5. For this network, it is even possible to see the topological structures in the node-link diagram (Figure 5(a)). Still, we use the adjacency matrix to select the four modules that can be observed (Figure 5(b)). The degree barchart exhibits one strong hub, which we select and highlight in yellow (Figure 5(c)). The selection of the hub triggers the automatic generation of layers around the hub as topological structures and a respective color assignment using a multi-hue luminance color map. The Icicle plot in Figure 7 allows for switching priorities between module and hub structures and for selection of the groups to generate the parameter-space visualization in Figure 6.

The parameter-space visualization in Figure 6 exhibits a pattern of module-hub interplay: For small values of parameter f, the Silhouette curves for hub layers are higher, but they decrease quickly with increasing values of f. At the same time, the Silhouette curves for modules are lower for small values of f, but increase at the beginning. Hence, the hub structures dominate over the modular structures for small values of f. However, with increasing values of f the hub is losing influence, while modules are gaining influence.

We validate this observation using the 2D dynamics-topology plots in Figure 7 for intervals P5-P7 selected in Figure 6. For small values of f, e.g., $f \in [0.0061583, 0.00626941]$ selected in P5, the layers around the hub synchronize, i.e., there are excitation waves that emerge from the hub and traverse through the network (Figure 7(a,b)). For increasing values of f, e.g., $f \in [0.191485, 0.191596]$ selected in P6, the modules start to synchronize, while the hub loses influence (Figure 7(c,d)). For large values of f, e.g., $f \in [0.62363, 0.623852]$ selected in P7, the influence of all topological structures diminish and eventually vanish (Figure 7(e)) .

4.3. Cat cortical network

In the last scenario, we investigate the cat cortical network. Again, we start by analyzing the topology to define meaningful topological groups: We use the adjacency matrix to observe and select modules and the degree barchart to select the largest hub (despite its degree not being significantly larger than those of others), see Figure 8. We use the Icicle plot in Figure 10 for selection of the groups to generate the parameter-space visualization in Figure 9.

The parameter-space visualization in Figure 9 exhibits that the Silhouette curves related to the modules are higher than those related to the hub, except for the curve of the bright-green module, which is lower than the curve of the second layer around the hub. However, the curve of the second layer appears to be rather noisy with high fluctations. When selecting a lower value of f, we can give modules higher priority in Figure 10(a) and observe that the modules synchronize, i.e., the modules are the dominant topological structures and govern the dynamics. It can be observed that the synchronization of the three modules appears until $f = 0.577956$. When changing the Icicle plot such that the hub layers are prioritized, these topologicals structures do not synchronize, see Figure 10(b). Since the hub was not so dominant, it is a valid assump-

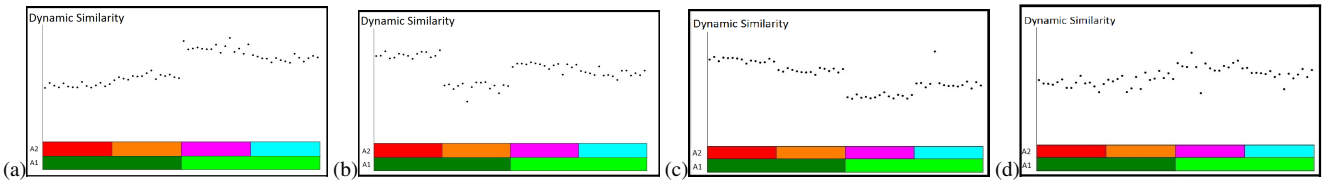

Figure 4: *Relating topology to dynamics for increasing parameter ranges (a) P3, (b) P4, (c) P1, and (d) P2 selected in Figures 3 and 2. For small values of f, the modules are dominant (a), for middle-range values the submodules become dominant (b,c), and for large values the modular structures lose their influence (d).*

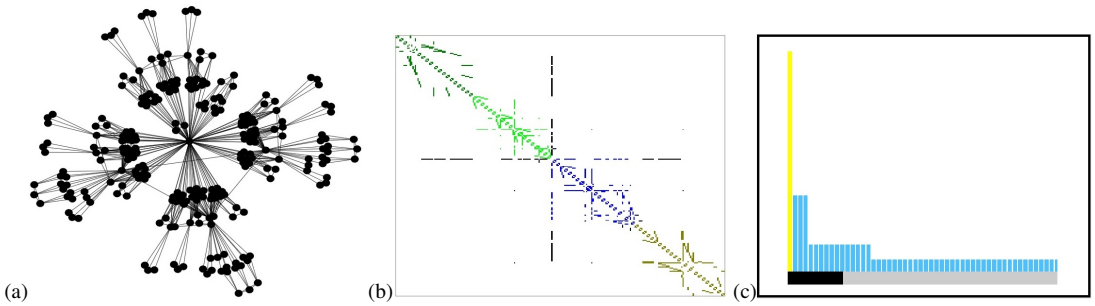

Figure 5: *Network with modules and hubs shown (a) as a node-link diagram, (b) in an adjacency matrix, and (c) with the degree barchart. Modules are selected in the adjacency matrix (4 colors), while the largest hub is chosen in the degree barchart (yellow color). Layers around the hub represent topological structures encoded with a multi-hue luminance color map: - hub, - 1st layer, - 2nd layer, - 3rd layer, - 4th layer.*

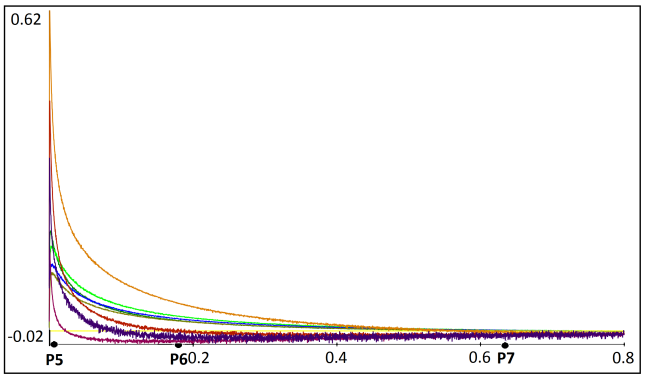

Figure 6: *Parameter-space visualization for topological structures selected in Figure 5. Silhouette curves show higher synchronization of hub layers for small f, higher synchronization for modules in middle-range f, and low synchronization of topological structures for large f. P5 marks interval $[0.0061583, 0.00626941]$, P6 interval $[0.191485, 0.191596]$, and P7 interval $[0.62363, 0.623852]$ for further investigation.*

tion that other hubs may have some influence, as well. We looked into the subsequent five largest hubs, but made the same observations. Hence, we can conclude that for the cat cortical network the three modules are governing the dynamical process for values of $f < 0.577956$. For larger values of f, all topological structures lose their influence, see Figure 10(c).

5. Discussion and domain expert opinion

As detailed above, our visual analytics approach allows us to interactively explore the relationship between network architecture and dynamics with an emphasis on collective dynamical states involving a subset of nodes of the network. The novel interactive visualization approaches incorporated in this toolbox guide the users in their search for fundamental principles relating network topology and dynamical features.

Our approach is the first to allow for an interactive analysis of the parameter space of a network dynamics simulation ensemble. In particular, we allow for the joint analysis of multiple topological features that can be defined and modified interactively. We document that even the interplay of topological features can be examined.

Our emphasis is on excitable dynamics, with a special focus on network architectures and dynamical properties relevant to computational neuroscience, as exemplified by the hierarchical networks (see [BS09] and [BBV*08] for a corresponding discussion in neuroscience) and the dynamical patterns of modular synchronization or wavelike activity (see [ZZZL*07], [ZZZ*06] and [MLHH08] for a corresponding discussion in neuroscience).

From the requirement analysis to the development of the system, our efforts were accompanied by a domain expert who has been working in the field of Network Science with application in Systems Biology for more than 20 years. His background is on studying correlations in term of biological self-organization in biological systems on different scales, ranging from genomes to interact-

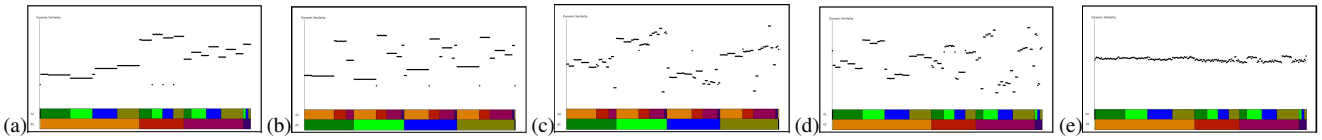

Figure 7: *Relating topology to dynamics for increasing parameter ranges (a,b) P5, (c,d) P6, and (e) P7 selected in Figures 6. Priorities for hub layers and modules are swapped interactively to examine both. For small values of f, the hub is dominant (a,b), for middle-range values the modules become dominant (c,d), and for large values the topological structures lose their influence (e).*

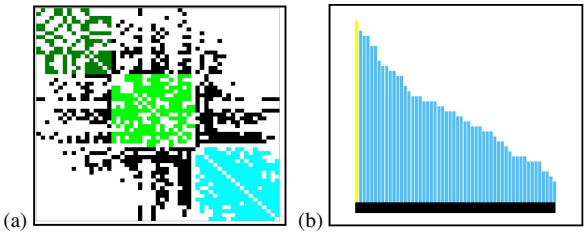

Figure 8: *(a) Adjacency matrix and (b) degree barchart of the cat cortical network are used to select modules and largest hub, respectively. Layers around the hub are encoded with a multi-hue luminance color map: - hub, - 1st layer, - 2nd layer.*

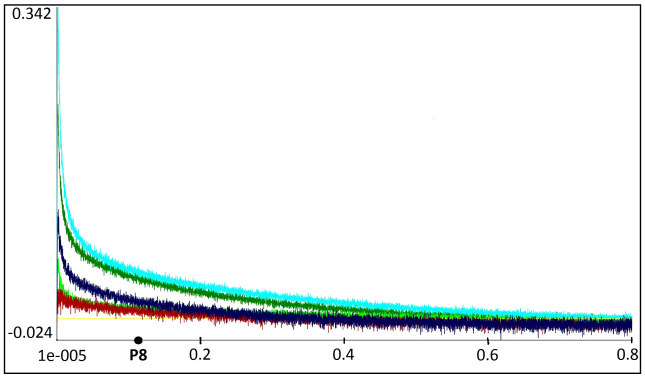

Figure 9: *Parameter-space visualization for $f \in [0.00001, 0.8]$ and topological structures selected in Figure 8. Silhouette curves of modules are high for most values of f (except for the bright-green module). P8 marks interval $[0.1141, 0.1146]$ for further investigation.*

ing cells. We also received encouraging feedback from practitioners in Computational Neuroscience. They considered our tool to be highly relevant and helpful, but also emphasized the need to interface our tool with the existing infrastructure in Computational Neuroscience (e.g., The Virtual Brain), thus suggesting a roadmap for our future work.

The result presented here on the topological scale selected by the noise level (or rate of spontaneous activity, f) in the system (see also the accompanying video) is an extension of the work from [MLHH08]. The fact that at different noise levels modules of different sizes (i.e., different topological scales) explain the activity patterns is reminiscient of the time-scale dependence of modular synchronization of phase oscillators as discussed in [ADGPV06]. This example illustrates, how our toolbox can facilitate the discovery of such relationships between topology and dynamics.

The scenarios presented here assumed a 1D parameter space, but they can principally be extended to multiple parameters. The sizes of the networks presented in this paper are typical for the given application. Still, the visual encodings (adjacency map, bar chart) scale sufficiently well to larger networks, while the other visual encodings do not depend on the network size. When looking at the scalability in the number of defined topological features, one limitation is the number of distinguishable colors, but this problem is diminished by our interactive analysis process. The same holds true for the parameter-space visualization, which may suffer from overplotting, but that can, again, be diminished by interactively selecting subsets.

Given that the generation of the ensemble may take a long time, it is feasible to also perform the computations of the distance matrix and the 1D t-SNE embedding in a pre-processing step. Afterwards, all analysis steps can be performed in an interactive session without significant delays, as it is documented by the accompanying video. To achieve low computation times, our tool integrates parallel computations of silhouette coefficients using the CUDA framework.

6. Conclusion

We presented a visual analytics approach for the analysis of for which parameter settings which topological features govern excitable network dynamics. Understanding the relationship between network architecture and dynamics is of upmost importance to a diverse list of application scenarios ranging from neuroscience and systems biology to social sciences and technology. The scenario outlined above is generic.

The discovery of novel relationships between network topology and dynamics is an important research trend in computational neuroscience. A decisive component of future development steps of this toolbox will, therefore, be to interface this tool with the main databases in computational neuroscience, thus allowing for upload of network topologies and experimentally observed activity patterns from these databases directly into our visual analytics toolbox.

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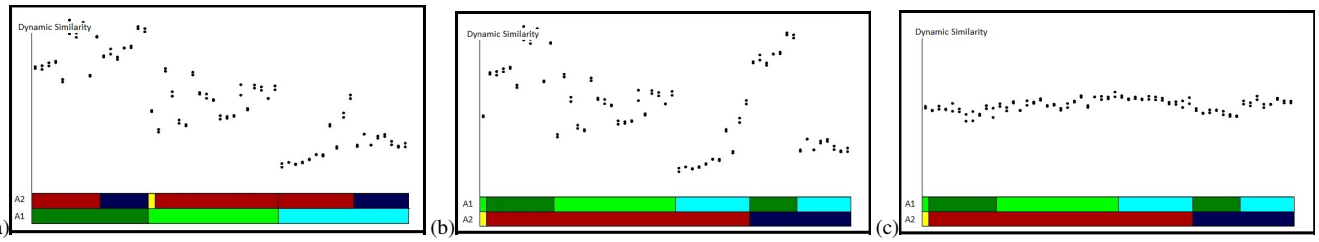

Figure 10: *Relating topology to dynamics for cat cortical network for ranges selected in Figure 9: (a) Modules synchronize for range P8 lower values of f, while (b) hubs do not. (c) Topology does not influence dynamics for $f > 0.577956$.*

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