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Short Papers

Projection-based Visualization of Dynamical Processes on Networks

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Abstract

Dynamical processes on networks play an important role in systems biology and statistical physics. To understand these processes, it is essential to understand which topological properties of the network are the main factors for the dynamics. We present a visualization approach that allows for such investigations. For visual encoding of the network topology, we use a node-link diagram. The nodes, however, are placed according to the dynamical processes. We use a projection method of the time series data to generate animations that maintain the mental map and exhibit the behavior of the dynamics. Suitable coloring schemes for the nodes encode the current values of the dynamics and individual nodes can be investigated with linked views to a time series plot. We present case studies to demonstrate that our approach is effective for the observation whether the dynamical processes follow the network topology.

1. Introduction

The complex networks found in biological systems and the various classes of random graphs (like [ER59], [BA99], [WS98], etc.) are typically high-dimensional objects that cannot be embedded in a low-dimensional (2D, 3D) space. Even in systems, where the nodes of the network are spatially arranged, like in many transportation networks, finding a functionally meaningful placing of nodes is non-trivial. In the German long-distance train connection network, for example, the travel time distances do not at all match geographical distances [FKW*10]. The purpose of typical network visualization algorithms is fundamentally different from our goals: We strive for network visualizations that are guided by dynamical data or functional information.

Dynamical processes on networks are defined in form of a graph $G = (V, E)$ with a set of vertices V and a set of edges $E \subset V \times V$ and the dynamics in form of dynamical variables $d(v,t)$ for each vertex $v \in V$ and time $t \in [t_1, t_n]$, where t_1 and t_n denote the start and the end of the described dynamical process, respectively. The dynamical processes are typically described by solving differential equations on each node or by state machines of the nodes, which update the dynamical variables of each node in each time step under the influence of adjacent nodes.

Many studies over the last few years, in particular in systems biology and in statistical physics, have provided dramatic examples, how a refined network layout can facilitate discoveries about the relationship between network architecture and network function (e.g., the comparison of topological modules with Gene Ontology (GO) classes or other functional categories [GA05], the embedding of gene networks in the genome [MGHM08, SHSS09], the analysis of effective networks derived from gene expression data under various cellular conditions [LBY*04, SGMH11], the distribution of real or simulated dynamical data across hierarchical levels [JBW*09, YG06, HJHL12]). In all these cases, the network layout was constructed for the purpose of highlighting a previously identified organizational principle. Our goal was to develop a novel visualization technique that by visual means provide insight into which topological features of the network may or may not be relevant for the development of the dynamics. The listed communities are the target users of the proposed system of visualizing dynamical processes on networks. Our methods needed to be developed and carefully calibrated by minimal models (like the two dynamical systems described in this paper), before they can be applied to more realistic models (e.g., of gene regulation, signal transduction, and metabolic pathways) or even to experimental data (in particular, microarray data, providing time courses of gene expression levels in a cell).

Our approach is based on a node-link diagram for display-

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ing the network, where a projection method is used for the node placement. The projection method projects from the n-dimensional space formed by the first n time steps into a 2D visual space by exploiting the similarities of the values of the nodes' dynamical variable for the n time steps of the dynamical process. The dynamical process is captured by an animation. Since dynamical variable values of previous time steps are included in the layout at any point during the animation, we maintain the mental map. During the animation, it can be observed how clusters form and how they relate to topological properties. The animation is supported by color encoding of the nodes with respect to the current dynamical variable value and by a linked view to a time series visualization. We demonstrate the effectiveness of our approach in case studies for two simple models for dynamical processes.

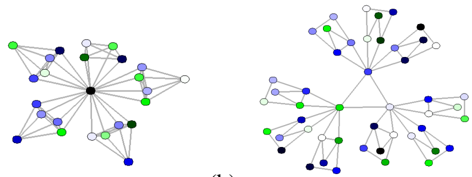
2. Related Work

Networks are commonly visualized using adjacency matrix visualizations or node-link diagrams. Node-link diagrams provide better means to display properties of nodes, which makes them preferable for our purposes. They are based on rendering the entities of the network as nodes and the relation between the entities as links (or edges). The main task to be solved is to position the nodes appropriately according to some design goal. Automatic layouts for node-links have been studied excessively in the graph drawing community [Tol96]. Different algorithms have been developed targeting graphs with certain properties. We refer to the surveys for graph drawing techniques on planar graphs [Wei01], orthogonal graph drawing [EFK01], multiple tree visualization [GK10], and drawing clusters and hierarchies in graphs [BC01] and to an annotated bibliography of algorithms [DBETT94]. A formal description of all graph drawing problems is given by Diaz et al. [DPS02]. The mentioned graph drawing problems are based on topological properties of the graph. Our objective, however, is more complex, as we want to develop layouts of the graph that reveal the dynamical processes of the graphs in relation to the topological properties. We also want to contrast our approach against dynamic graph drawing techniques. The goal of dynamic graph drawing is to visualize a graph in an animated fashion to show topological changes over time [Bra01]. We want to visualize dynamical processes on graphs, where the dynamical processes are reflected by the changing properties of nodes over time, while the topological structure of the graph is typically static.

In the visualization community, approaches for network visualization enhance the visual encoding (in the sense of graph drawing) with interaction mechanisms that allow for an interactive visual exploration and analysis of the graphs [HMM00, TAS09]. A comprehensive very recent survey on visual network analysis including visual encoding and interaction algorithms is given by von Landesberger et al. [vLKS*11]. Commonly, the graph analysis task is to investigate the relationships between entities in the graph and to assess the global graph structure. Our analysis is not based on the graph topology only, but on the dynamics on the graphs in relation to the topology.

3. Animated Node-link Diagram Based on Dynamical Processes

The graph $G = (V,E)$ is visually encoded using a node-link diagram. Hence, the topological structure is shown in form of edges that connect adjacent nodes. The current dynamical variable value $d(v,t)$ for a node $v \in V$ at time t is visually encoded using a color mapping. Figure 1 shows examples of graphs with different topology, where a force-based layout algorithm is used to depict the graph topology.



(a) (b)

Figure 1: *Node-link diagrams of graphs with different topology and color-coded dynamical variable values of a given time step. The layout of the graphs are solely based on topology using force-based positioning.*

To lay out the nodes of the graph with respect to the dynamical processes on the network, we investigate the similarities of the time series of the dynamical variable $d(v,t)$. The similarity or distance measure between two time series $d(v_i,\mathbf{t})$ and $d(v_j,\mathbf{t})$ for any two nodes v_i and v_j and time sequence $\mathbf{t} = (t_1,\ldots,t_n)$ depends on the encoding of the dynamical variable. Two common groups of dynamical variables exist: First, the dynamical variables may be categorical such that the distance measure becomes

$$dist(d(v_i,\mathbf{t}),d(v_j,\mathbf{t})) = \frac{1}{n}\sum_{k=1}^{n}\delta(d(v_i,t_k) \neq d(v_j,t_k)),$$

where

$$\delta(x) = \begin{cases} 1 & \text{if } x = \text{TRUE} \\ 0 & \text{otherwise} \end{cases}$$

Second, the dynamical variables may be numerical such that the distance measure may become the Euclidean distance. However, for the scenario investigated in our case study the dynamical variables actually represent phases $\in [0,2\pi)$ and the distance measure becomes

$$dist(d_i,d_j) = \frac{1}{n}\sum_{k=1}^{n}\sqrt{(\cos d_{ik} - \cos d_{jk})^2 + (\sin d_{ik} - \sin d_{jk})^2}$$

with $d_i = d(v_i,\mathbf{t})$ and $d_{ik} = d(v_i,t_k)$.

Based on these similarities between nodes, we project the time series $d(v_i, \mathbf{t})$ from the n-dimensional space into a 2D visual space. A well-known and well-established technique to do so is multi-dimensional scaling (MDS) [CC01]. MDS takes as input a matrix of pairwise distances like the ones established above and computes locations in a Euclidean space such that distances are preserved as much as possible. More precisely, we assign to each node v_i a 2D position $\mathbf{p}_i$ such that the positions of all nodes minimize the functional

$$\sum_{i<j} (\|\mathbf{p}_i - \mathbf{p}_j\|_2 - dist(d(v_i, \mathbf{t}), d(v_j, \mathbf{t}))^2.$$

To show the dynamical processes on the network, we develop an animation that changes the positions $\mathbf{p}_i$ of nodes v_i over time. In each time step $t_k = t_1, \ldots, t_n$, we apply an MDS step to compute the new positions. To maintain the mental map during the animation we use the entire time series from starting point t_1 to the current point in time t_k for building the distance matrix. Hence, the animation has a memory and point locations only change positions slightly with respect to the preceding layout. Due to the nature of MDS, it may happen that the entire layout is flipped over, which can easily be fixed by checking the coherence of two successive time steps and potentially perform sign changes.

4. Color Encoding

The color encoding of the nodes is performed with respect to the current dynamical variable value $d(v_i, t_k)$ of each node v_i. The mapping depends, again, on the encoding of the dynamical variable. In case of categorical values, we assign distinct and clearly distinguishable colors to the different categories. For the scenario shown in the case study, we have three categories, which are mapped to red, blue, and yellow, respectively. In case of numerical values, one can assign a standard continuous color map. Since our scenario deals with phases, the color map shall be continuous and cyclic, i.e., it shall assign the same values to phases 0 and 2π. We achieve this by using a four-color scheme that assigns white to phase 0 and 2π, respectively, blue to phase $\frac{\pi}{2}$, black to phase π, and green to phase $\frac{3\pi}{2}$. For other phases we obtain the colors by interpolating luminance values. The color map basically consists of a blue and a green luminance color map, which can be attached to each other continuously at the luminance minimum (black) and maximum (white), respectively. Figure 1 is using this color mapping scheme.

5. Time-series Visualization

We also provide a linked view to a time series visualization. Individual nodes can be selected and are highlighted in both the nodelink diagram and time series visualizadtion. The time series visualization depicts the dynamical variable values of all nodes over time in 2D Cartesian coordinates. For the scenario of dealing with phases, 2D polar coordinates can be used, where time increases towards the origin and the phases are located at the respective positions on a circle. Figure 2 shows the two layouts for time series visualization, where the radial layout is a hyperbolic one.

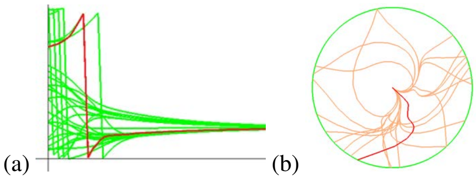


Figure 2: *Time series visualization is linked to the node-link diagrams. (a) Using 2D Cartesian coordinates. (b) Using 2D polar coordinates, where time increases towards the origin.*

6. Case Study

We applied our visualization methods to two different types of dynamical processes and each of them to networks with different topologies. The first dynamical process we have been investigating is that of synchronization of nodes within a network. A widely used model is the one by Kuramoto, where the nodes represent a population of phase oscillators that are coupled through phase differences [Kur84, Kur03], which has been studied on graphs, e.g., by Arenas et al. [ADGPV06]. The following differential equation is used to simultaneously update the phase values $d(v_i, t)$ of each node v_i at each time step:

$$\frac{\mathrm{d}\,d(v_i, t)}{\mathrm{d}t} = \varepsilon \sum_j A_{ij} \sin(d(v_j, t) - d(v_i, t)),$$

where $A = (A_{ij})$ is the adjacency matrix that captures the network topology in form of binary entries and ε is a global parameter inducing a coupling strength. The process tries to synchronize connected nodes, i.e., it tries to assimilate their phase values. We first applied this dynamical process to the network shown in Figure 1(a). The network consists of five fully connected groups that are connected to a hub. Four of the five groups have a node that is not directly connected to the hub. The respective time series are shown in Figure 2. We run the dynamical processes multiple times with different random initial dynamical variable values and average the time series for each node. The result of our animation is depicted in Figure 3. It can be observed how the five fully connected groups and the hub start to separate over time. Moreover, the nodes that are not directly connected to the hub are placed more distant from the hub than the directly connected nodes of the same group. Hence, the dynamics follow the topology and it can be concluded that the hub is the main structural feature of the dynamical process.

Next, we applied the same dynamical process to other networks including the one shown in Figure 1(b). The main topological structure of the network is given by three groups that are coupled via a hub for each group. At the hubs, each group splits into three subgroups. The animation shows that it takes significantly longer to build a clear structure, but that

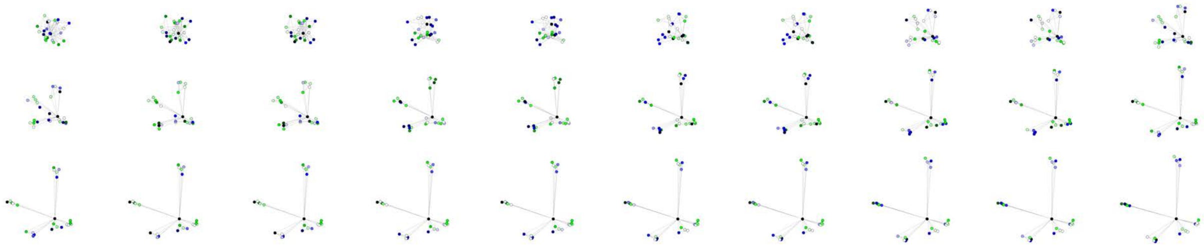


Figure 3: *Animation of node-link diagram based on dynamical processes with mental map. Vertex positions for all nodes v_i in the 30 figures are computed using MDS on time series $(d(v_i,t_k))_{k=1}^n$ for $n = 1,\ldots,30$, respectively. It can be observed that the topological structure (Figure 1(a)) clearly triggers the dynamical process.*

the main topological structure is again dominant. The triangle formed by the three hubs governs the process, see Figure 4(a) for time step t_{99}. However, here the hubs do not separate clearly from the three subgroups within the respective groups.

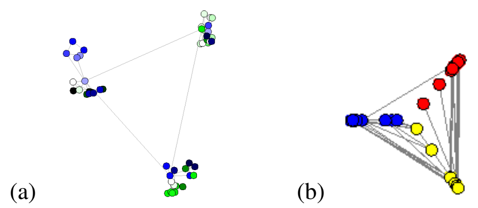


Figure 4: *Results for the network in Figure 1(b): (a) Time step t_{99} of animation for synchronization process. (b) Time step t_{45} of animation for excitable networks.*

The second dynamical process that we investigated was that of excitable networks, which plays an important role in biological modeling [MLHH08]. Each node is in one of the three states 'susceptible', 'excited', or 'recovering'. A 'susceptible' node enters the state 'excited' in the next time step, if at least one of its adjacent nodes is in the state 'excited'. Moreover, even if no adjacent node is 'excited', the 'susceptible' node may still get 'excited' with a certain probability, called the spontaneous excitation rate (here, we chose a spontaneous excitation rate of 0.1). An 'excited' node always enters the state 'recovering' in the next time step. A 'recovering' node enters the state 'susceptible' in the next time step with a certain recovery probability (here, we chose a recovery probability of 0.9). We applied this dynamical process to the networks shown in Figure 1. Figure 5 show four consecutive time steps of the animation when applied to the network shown in Figure 1(a). It can be observed that the three states govern the process and that network topology does not play the main role. Note that other influences of topology on dynamics may still exist. A similar observation can be made when applying the approach to the network shown in Figure 1(b). One time step is shown in Figure 4(b).

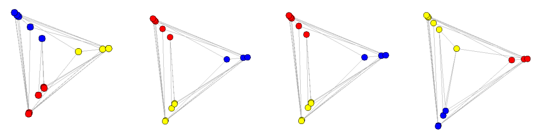


Figure 5: *Four consecutive time steps of animation for excitation networks on network in Figure 1(a). No topological structures appear.*

7. Discussion

We have compared our results with two other types of visualizations: First, we took a static graph layout based on the network's topology and animated the colors of the nodes over time. Figure 1 shows one of the time steps. As we can see from Figure 3, there are nodes with very similar time series whose current dynamical variable values are nevertheless rather different. Hence, it was impossible to see any emerging structures from a color animation over a static graph.

Next, we looked into a dynamic force-based layout, where the node locations are animated based on the similarity of the current dynamical variable values. It turned out to be impossible to maintain a mental map and positions changed so quickly, in large number, and in an uncoordinated fashion that no structural behavior could be observed.

8. Conclusion

We have presented a visualization method for dynamical processes on graphs based on an animation of node positions. The node positions are obtained using an MDS approach on the time series, which allows for an animation that maintains the mental map. We have shown for different dynamics and different topologies that our visualization approach can be useful to draw conclusions about the relationship between network topology and dynamical processes for minimal models.

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