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Cartographs enable interpretation of complex network visualizations

Networks offer a powerful visual representation of complex systems. Cartographs introduce a diverse set of network layouts for highlighting and visually inspecting chosen characteristics of a network. The resulting visualizations are interpretable and can be used to explore complex datasets, such as large-scale biological networks.

The problem

Networks are used to represent and investigate complex systems across virtually all fields of science[1]. Their widespread adoption is due to the versatile computational and analytical tools that networks offer, as well as their ability to visually represent information in an intuitive manner. The simple, yet powerful portrayal of nodes and links enables a seamless back and forth between conceptual, 'back-of-the-envelope' sketches, and network depictions of real systems, thus facilitating both theory development and concrete data interpretation. However, a critical roadblock in this process, in particular for larger, more complex networks, is the lack of network layouts that allow for a straightforward interpretation of observed visual patterns. Indeed, standard layout algorithms are prone to generating proverbial 'hairball' visualizations that often obscure network structure, rather than elucidate it. As a result, it is often not possible to visually recognize connection patterns that can be analytically proven to be present in a particular network, or, conversely, to trust visual patterns to truly reflect an intrinsic structural feature of a network.

The solution

Our work presents a method of using dimensionality reduction techniques for mapping network information directly into node positions (Fig. 1a). We introduce four network maps, which we termed cartographs, in two and three dimensions (Fig. 1b). Recent advances in the field of dimensionality reduction[2] allow us to compute cartographs for networks with thousands of nodes within a few minutes or less on a standard laptop computer. Any network information can be encoded and visualized in this fashion, including internal information, such as the structural importance of a particular node within the network, but also external node annotations, such as the similarity of nodes with respect to a given functional characteristic.

We tested our approach on simple model networks and on the large-scale interactome network of all known molecular interactions among human proteins, consisting of over 16,000 nodes and 300,000 links. We found that cartographs can visually represent well-known interactome characteristics, such as the close relationship between the biological role of a protein and its centrality within the network[3]. Similarly, we show that cartographs can be used to visualize connection patterns among a group of proteins associated with the same disease, which are difficult to decipher using conventional methods. The flexibility of our framework allows users to custom-tailor network visualizations for a specific application. For example, we designed a 3D interactome layout specifically for inspecting the biological functions of candidate genes that are suspected to cause rare diseases[4]. Finally, we show that our layouts can be incorporated into a virtual reality (VR) network exploration platform[5], thereby facilitating the visual inspection of large networks such as the interactome (Fig. 1c).

Future directions

The addition of interpretable visualizations to the toolbox of network analysis methods offers new opportunities for investigating the wide range of systems that can be represented as networks. We envision our framework to be part of an iterative data exploration workflow in which visual inspection enables the generation and subsequent testing of novel hypotheses related to relationships between the structure of a network and its functional implications. The possibility of combining and jointly displaying various structural and functional network data is perhaps the most powerful feature of our framework for concrete applications.

Since our framework is designed to explicitly highlight a chosen network characteristic, any observed pattern needs to be carefully and independently evaluated to conclusively show its presence in the underlying data. Our framework relies on dimensionality reduction techniques and is therefore subject to the same challenges as them, such as the emergence of spurious patterns, but also computational performance, or robustness towards variations in the parameters of the respective algorithms. Furthermore, the interpretability of any data visualization is constrained by the media on which it is displayed. Static images are limited to smaller network sizes than our new interactive web application and VR platform offer.

A fundamental challenge in exploring large datasets is to connect the analytical power of computational tools with human capabilities, like intuition, creativity, and the ability to link experience with both specialist and broad general knowledge. We believe that network visualizations, combined with advanced data display technologies like VR, have great potential for helping establish this connection.

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EXPERT OPINION

"This interesting paper presents a great way to visualize large networks using dimensionality reduction". **Steven Gygi, Harvard Medical School, Boston, USA**

FIGURE

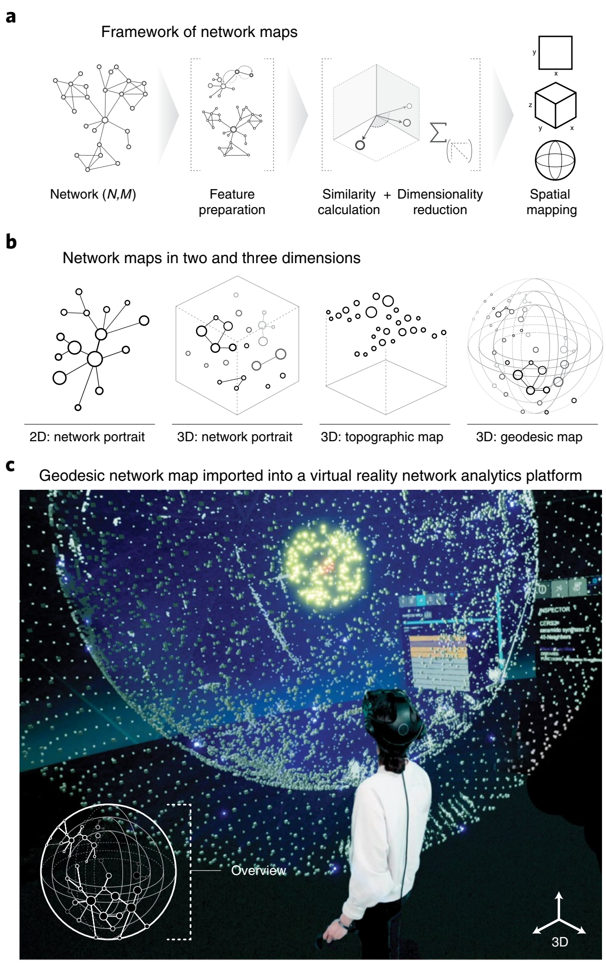

Fig. 1 | Interpretable network visualizations. a, Network characteristics to visually emphasize are encoded as node features and then mapped into node positions in 2D or 3D using dimensionality reduction methods. **b**, Four types of network maps provide a diversity of visualizations for a wide range of applications. **c**, A user exploring a protein interaction network in virtual reality (VR)[5]. Proteins with specific biological functions are arranged on different spherical layers.

BEHIND THE PAPER

Since I started working on complex networks, some 15 years ago during my PhD, the ability to produce meaningful layouts for large networks has been a constant challenge. Like many of my colleagues, I grew more and more skeptical as to whether visual network exploration could be achieved in a systematic fashion. After all, in the absence of a suitable framework for interpretable layouts, it was not clear how exactly an iterative workflow of visual hypothesis generation and rigorous evaluation should look. I believe that the framework we propose finally offers a solution to this key challenge; it has certainly changed my perspective on the power of network visualization and I hope that other researchers will find it equally useful. **J.M.**

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FROM THE EDITOR

"Interpreting complex networks is crucial to develop new knowledge from complex systems, such as large-scale biological networks. The tool presented here will enable the full potential of network visualization to be realized. It is an iterative workflow to generate visual hypotheses and can be integrated into a VR platform. I hope that it will become a useful resource to guide effective searches for meaningful information in large-network analysis." **Jie Pan, Associate Editor, *Nature Computational Science***.