Geometric and Topological Inference for Deep Representations of Complex Networks

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ABSTRACT
Understanding the deep representations of complex networks is an important step of building interpretable and trustworthy machine learning applications in the age of internet. Global surrogate models that approximate the predictions of a black box model (e.g. an artificial or biological neural net) are usually used to provide valuable theoretical insights for the model interpretability. In order to evaluate how well a surrogate model can account for the representation in another model, we need to develop inference methods for model comparison. Previous studies have compared models and brains in terms of their representational geometries (characterized by the matrix of distances between representations of the input patterns in a model layer or cortical area). In this study, we propose to explore these summary statistical descriptions of representations in models and brains as part of a broader class of statistics that emphasize the topology as well as the geometry of representations. The topological summary statistics build on topological data analysis (TDA) and other graph-based methods. We evaluate these statistics in terms of the sensitivity and specificity that they afford when used for model selection, with the goal to relate different neural network models to each other and to make inferences about the computational mechanism that might best account for a black box representation. These new methods enable brain and computer scientists to visualize the dynamic representational transformations learned by brains and models, and to perform model-comparative statistical inference.

CCS CONCEPTS
• Theory of computation → Machine learning theory; • Human-centered computing → Visualization; • Networks → Network properties.

KEYWORDS
representation learning, network inference, applied topology

1 INTRODUCTION
In this work, we propose a series of statistical inference techniques to compare complex networks in terms of summary-statistical descriptions that capture their topological and geometric structure. Consider a set of $N$ individuals in a social network. Their relationships can be characterized by their pairwise degrees of separation in the network, by dissimilarities of their profiles, or by geographical distances between their homes. Each of these topological and geometric summaries can be expressed in a square matrix of pairwise relationships. The same summary statistics can be used to characterize representations of $N$ visual images in a layer of a neural network or in a cortical area of human brain, indicating to what extent different images are dissimilar in multivariate neural representational space (geometry) and which stimuli share neighbor relationships (topology) in that space. Based on persistent homology, prior work in topological data analysis has enabled expressive graph visualizations. Here we focus on geometric and topological descriptors for formal inferential comparisons between multiple representations or networks. These methods enable us to infer, for example, to what extent geographical proximity and profile similarity are related to the degrees of separation in a social network, and whether proximity is significantly more related to the degrees of separation than profile similarity. Similarly, these methods support assessing to what extent the representation of photos in a neural network is similar to the representation in another neural network or a brain region, and whether one of the networks provides a better model of the brain representation [22].

To integrate geometric (distance-based) and topological (graph-based) characteristics and embed both in a consistent inferential framework, we introduce a nonlinear monotonic transformation of distances, which provides a family of statistics combining geometric and topological information. Our applications include neuroscience [23], collaborative filtering and independence testing [21].

Other than graph-based network properties, we also investigate higher-order topological inference and information-theoretical measures. For instance, similar to the evolving nature of social networks and preferential graphs, in single-cell genomics, the lack of a formal link between cell-cell cohabitation and its emergent dynamics into cliques during development has hampered our understanding of how cell populations evolve across time. We introduce higher-order simplicial structure as a new summary statistic, and discover that these networks contain an abundance of cliques of single-cell profiles bound into cavities that guide the emergence of more complicated habitation forms [15, 19]. To further disentangle information flow, we develop a mathematical filtration technique to compute nerve balls in a dual metric of space and time [20] and a information-theoretical measure among network modules [16, 18].
2 PROBLEM SETTING AND SIGNIFICANCE

This work aims to solve the following two analytical problems.

Aim 1: Develop novel analyses of representational geometry and topology. Visualizations of neural dynamics can reveal representational transformations and, thus, neural computations. Classical studies have used linear dimensionality reduction methods (e.g., PCA [27], jPCA [4], dPCA [7]), tensor components analysis [34], “hypothesis-guided” dimensionality reduction (HDR) [12] to embed high-dimensional trajectories of neural population activity in visualizations. However, linear dimensionality reduction may distort the geometry, collapsing dimensions that contribute to the discriminability of representational patterns. We develop extensions of multidimensional scaling (MDS) [1] and TDA [2] for visualization of network dynamics that are optimized to accurately reflect the representational geometry and topology. These methods provide an important complement to existing techniques by forgoing the simplicity of a linear subspace in exchange for a better reflection of the degree to which information about stimuli and task-relevant latent variables is represented for readout by downstream modules.

Aim 2: Investigate the representational dynamics and information of recurrent networks. Recurrent neural nets (RNNs), as the generalized form of neural nets, are not only useful for learning the latent structure of sequences, but also provide a candidate computational model for how the human and animal brains perform a variety of tasks. As an RNN engages a dynamic world, information about the recent history of inputs is accumulated, dynamically compressed, and propagated along the cyclic computational graph. Classical studies in dynamical modeling recently supported a direct mathematical link of recurrent networks with other popular deep learning architectures such as residual network (ResNet) and convolutional networks (ConvNet) [14]. Investigating the representational dynamics of RNNs in information flow and accumulation within and across layers is critical to deep learning theory and to the development of better architectures that provide appropriate inductive biases to enable a faster learning and faster dynamic convergence during inference. We explore a broad set of summary statistics (e.g., SVCCA [28], CKA [8] and the novel geo-topological summary statistics from Aim 1) and visualization methods.

Different summary statistics are then evaluated by an objective benchmark that reflects the degree to which they enable accurate inferences about data-generating model, when data are sparsely sampled and models are trained from different random seeds than the data-generating one. The goal is to select the best descriptors to capture underlying invariant aspects of representational geometry and topology along the temporal dimension of RNN dynamics (across unfolded time steps, layers, learning stages and task states).

Impact will be threefold: (1) Understanding the representational signatures of RNNs help us compare and improve architectures, which enable engineering advances. (2) Visualizations reveal the latent task-related states, contributing to explainable AI by providing a more abstract functional description of the computations performed by RNNs. (3) These new methods enable us to test RNNs as models of dynamic computations in brains. This addresses a major challenge in computational neuroscience: how to connect increasingly rich and detailed measurements of brain activity to increasingly complex and powerful neural net models?

3 METHODS

We introduce a range of new analysis and visualization methods.

3.1 Develop novel analyses of representational geometry and topology

The representational geometry is defined by the representational dissimilarity matrix (RDM) as the summary statistic or, equivalently, by the second moment of the activity profiles. The RDM constitutes an intermediate level summary statistic: It discards some of the information contained in the distribution of activity profiles, but retains more information than a linear decoding approach. Here we explore discarding additional information and considering the representational topology alongside the representational geometry.

There are two motivations for exploring this, one theoretical and one data-analytical. From a theoretical perspective, the local geometry determines which input stimuli the representation renders indistinguishable, which it discriminates, but places together in a cluster, and which it places in different neighborhoods. The global geometry of the clusters (whether two stimuli are far or very far from each other in the representational space) may be less relevant to computation: In a high-dimensional space a set of randomly placed clusters will tend to afford linear separation of arbitrary dichotomies among the clusters [11, 30] independent of the exact global geometry. Like a storage room, a representational space may need to co-localize related things, while the global location of different categories may be arbitrary. From a data-analytical perspective, conversely, small distances may be unreliable given the various noise sources that may affect the measurements. From both theoretical and data-analytical perspectives, it seems possible that focusing our sensitivity on a particular range of distances turns out to be advantageous because it reduces the influence of noise and/or arbitrary inter-individual variability (e.g., of the global geometry) that does not reflect computational function.

We introduce a novel approach called representational geo-topology analysis (RGTA), which builds on the literature on topological methods (e.g., persistent homology [35], TDA mapping [2]). The utility of a focus on topology derives from the idea of persistence, where unreliable features are discarded to reveal the underlying structure in the data. In order to summarize the idiosyncrasies of individual brain mechanisms and highlight the representational properties that are key to their computational function, we would like to find an optimal upper distance threshold $l$ above which we consider stimuli distinct, but do not consider differences between distances meaningful (i.e., the stimuli are disconnected in the graph capturing the topology at the appropriate scale). In order to suppress noise, we would like to find a lower threshold $u$ below which we consider stimuli as co-localized (i.e., the stimuli collapse into the same node in the graph). Between two thresholds we place a continuous transition to retain some geometrical sensitivity in the range where it matters (Figure 1).

Optimizing representational geo-topological analysis for RNNs. When applying RGTA to a multi-layer neural network, we will optimize thresholds $l$ and $u$, so as to best select the data-generating model representation. Model selection is based on a comparison of the RGTA summary statistics estimated from data generated by some model to those from separately trained instances of the same and different network architectures (different random
We can efficiently estimate the inter-module interaction between TDA applications usually focus on the low-dimensional graph visualization methods (notably PCA and supervised variations including in static images. Classical studies have used dimensionality reduction to find a single 2d or 3d linear subspace in which to view the trajectories. This approach of linear-subspace trajectories is well motivated by its simplicity and interpretability. Certain distinctions may be collapsed, but an advantage is that the approach equally represents within-time-point and between-time-point relationships among representational patterns. This enables us to visualize neural population response for even a single experimental condition as a trajectory. We then align the embeddings of learned transformations; (c) effect on the distance matrices.

Figure 1: Representational Geo-Topology Analysis (RGTA). (a) nonlinear monotonic transform of distances; (b) a family of transforms; (b) interpretations of learned transformations; (e) effect on the distance matrices.

Figure 2: Pipeline of 2d+time representational dynamic analysis.

3.2 Investigate the representational dynamics and information of recurrent networks

Neural computations unfold over time. Visualizations of network dynamics can help us understand how representations are transformed and gain insight into the computational process. Static visualizations of individual time frames can be animated by applying them in a time-windowed style to render neural dynamics as a movie. However, it is also important to visualize neural dynamics in static images. Classical studies have used dimensionality reduction methods (notably PCA and supervised variations including

\[ u = \max \text{, i.e., the original RDM.} \]

- Time-point relationships among representational patterns are untangled in the high-dimensional representation [31]. This motivates alternative visualization methods that aim to represent the pairwise discriminabilities of the representational states (e.g. of sensory stimuli). MDS offers one such method, which optimizes the accuracy with which pairwise distances in the high-dimensional space are reflected in the visualization. We develop extensions of MDS for visualizing dynamic representational geometries. The analyses of representational dynamics will use the summary statistics of geometry and topology developed in Aim 1. We can relax the requirement of MDS for models to accurately reflect the geometry (e.g. pairwise distances) and require only that models accurately reflect the topology (e.g. neighborhoods) of representational space.

Ride along with a dynamic representational geometry. Einstein famously imagined riding alongside a beam of light. This thought experiment, a mental visualization, rendered stationary the most rapid dynamic process, and was a major inspiration that contributed to a scientific breakthrough. To visualize neuronal population dynamics, we may similarly choose either a static or a moving reference frame. Neural population dynamics [4, 6, 25] are often visualized using dimensionality reduction methods such as PCA and its extensions [4, 7, 13, 25] to find a single 2d or 3d linear subspace in which to view the trajectories. This approach of linear-subspace trajectories is well motivated by its simplicity and interpretability. Certain distinctions may be collapsed, but an advantage is that the approach equally represents within-time-point and between-time-point relationships among representational patterns. This enables us to visualize neural population response for even a single experimental condition as a trajectory.

Here we introduce an alternative approach, in which we travel along with the ensemble of high-dimensional points that correspond to different experimental conditions (e.g. different stimuli or different movements performed by the animal). Rather than embedding all neural activity patterns across all time points in a single space, we first seek to represent the relationships between the patterns separately at each time point. We then align the embeddings across time points so as to minimize motion of the ensemble as a whole and render more apparent the changes of the representational geometry or topology, i.e. which stimuli become distinct and which collapse and how their global distances develop. Any visualization method including linear subspace methods and the methods from Aim 1 could be used to obtain a separate configuration for each time frame. To illustrate the concept of a dynamic visualization with a moving frame of reference, let us consider MDS.
MDS is a natural choice for visualizing geometries because it minimizes the distortion of the distances in the visualization (using the metric stress cost function here). The MDS cost function explicitly penalizes the collapsing of points that are distant in the original space, e.g., neural patterns that represent distinct states [31].

Figure 2 shows the sequence of steps of the proposed procedure. First each time frame of neural activity is analyzed separately. This could involve, for example, spike counts performed in a temporal sliding window to obtain a neural population activity pattern for each experimental condition. Second, for each time frame, the representational dissimilarity is estimated [9] for each pair of experimental conditions and assembled in the representational dissimilarity matrix (RDM). Stacking these RDMs along the time dimension results in an RDM movie. Third, each RDM is separately subjected to MDS to obtain, for each time frame, a 2d or 3d configuration of the points for visualization. Fourth, the configurations are aligned to each other using Generalized Procrustes Analysis (GPA), and finally, the aligned configurations are presented together. The alignment implements the moving frame of reference, which minimizes the motion of the ensemble as a whole in the visualization from one time point to the next. We can present the low-dimensional embedding of the dynamics as a movie (using visualization time to represent neural activity time) or as a static figure. For a static figure, we must choose how to indicate the time frame. In Figures 2 and 3, we designate one dimension of the visualization space as representing time and used the remaining two orthogonal dimensions for the relationships among stimuli within a time frame.

Assessing model similarity of RNNs in different tasks. Following a similar experimental setup as [24], we train populations of thousands of networks, with different variants of RNN architectures such as RNN, Long-Short-Term-Memory (LSTM) [5], Gated Recurrent Unit (GRU) [3] and bidirectional versions of the above [32], and characterize their nonlinear dynamics. We consider a range of neuroscientifically and computationally motivated tasks: signal-transform tasks such as frequency-cued sine wave and K-bit flip-flop [33], computer vision tasks such as object classification, and logic tasks such as time-windowed logic gates (e.g. XOR). To select the best statistics for the model similarity, we compare and evaluate several metrics: (a) representational-space-based metrics (of dimension $n_{\text{cond}} \times n_{\text{channel}}$) such as SVCCA, CKA and projection weighted CCA (PWCCA) [26], and (b) RDM-based metrics [10] (of dimension $n_{\text{cond}} \times n_{\text{cond}}$) such as cosine distance, Euclidean distance, and correlation distance with Pearson’s $r$, Spearman’s $\rho$, and Kendall’s $\tau$. The model pairs being considered are different RNN networks with different architectures, different RNN layers, the same layer but at different time steps, RNN networks in different training stages, as well as RNNs trained in one task and tested for generalization to a different task.

Assessing model-brain similarity, based on neural population activity data. The methods will be applied to a wide range of neural population activity data sets, acquired in different species (mice, marmoset monkeys, macaque monkeys) during a variety of tasks (visual perception, odor discrimination, motor tasks). We pursue both data-driven visualizations of neural population dynamics and model-driven analyses, where the aim is to adjudicate among alternative RNN models as models of the dynamics and computational function of biological neural networks.
Topological simplicial analysis with temporal filtration. In [15, 19], we propose a topological simplicial analysis (TSA) pipeline as an exploratory inquiry to solve these two challenges: (1) with the algebraic geometry’s definition of forming higher-order simplices, we can potentially interpret that cliques of higher orders indicates operational units of higher order; (2) with the bootstrapping techniques to sample from the data points collected at each sub-level, we can scale the analysis to large single cell datasets and compare groups of cells quantitatively. In addition, in [20] we heuristically define a technique to extract the temporal skeleton of the developmental processes, called temporally filtered TDA, and show that the developmental trajectories of cells can be better revealed in this approach comparing to traditional TDA mapping.

Information flow within network modules with minimum description length. To put this direction in perspective, we mention that this line of work is a series of three. The entry point is [16], where we propose a perspective to understand neural network optimization as a partially observable model selection problem. In our subsequent work [18], we introduce the details of how to approximate the minimum description length (MDL) between neural network layers and demonstrate that using MDL as the regularity information is useful, from an engineering angle, for neural networks to learn from certain input data distributions. By comparing with other theoretical tools such as mutual information, we envision it as a tool to understand how information propagated between network modules, a venue not widely explored previously, as in [17, 18]. In our third stage, we aim to bridge the information-theoretical tool (e.g. MDL) with the group actions. We have this intuition that traditional usage of mutual information mostly deals with statistical association, while MDL quantifies the efficiency of the transformation function in the communication system, i.e. the degree to which the groups are symmetric. If we can formulate the theoretical grounds for this intuition, we might be able to show that over the time of the optimization process, the transformation function (as a manifold) converges to an invariant geometric structure, reflected by a higher and higher communication efficiency.

5 CONCLUSION

In summary, we propose a series of statistical inference techniques to compare complex networks in terms of summary-statistical descriptions that capture their topological and geometric structure, in order to characterize the temporal evolution of dynamic networks and information flow of computational graphs. There are four main research outcomes: (1) an adaptive independence test with geometric transformations; (2) a topological simplicial framework for high-throughput time-series data; (3) the representational similarity analysis for robust model inference of artificial and biological neural nets; (4) a MDL estimate to quantify information flow among network modules. Future work include applying these techniques on other complex networks (e.g. social networks and recommendation systems) and providing physical interpretations for the geometric and topological objects emerged from these complex networks.

ACKNOWLEDGMENTS

I thank Dr. Niko Kriegekorte, who advised and assisted the study.

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