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Algebro-topological invariants in network theory

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Abstract. The dynamical evolution of a network is strongly associated with its pattern of internal connections [2, 5]. The lack of periodic patterns in the vast majority of biological networks, and in recurrent neural networks in particular, makes it difficult to determine this correlation from a theoretical and formal approach, other than relying on descriptive statistical parameters when trying to describe the network dynamics [3]. Algebraic topology provides us with invariants that are a powerful tool to understand the structure of abstract spaces and can also defined for graphs. We propose to apply those invariants to network science. Even simple invariants such as the Euler characteristic or the Betti numbers can provide us with valuable insight about the structure of a network and its connectivity, complementing measures such as centrality of nodes. We introduce certain topological invariants and use them to apply methods from algebraic topology in an attempt to characterize and classify networks and reveal their internal structure, looking in particular at recurrent neuronal networks, where we can use such invariants to detect the topological structure of the network and its activation patterns.

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1. Introduction

The main interest of Algebraic Topology is to study and understand spatial structures. In Network Science we want to understand and describe the shape and the structure of particular objects, namely networks, and the application of the tools provided by Algebraic Topology can give us a very powerful framework. We shall introduce certain topological constructions that produce invariants encoding the structure of networks. These constructions are completely general and can be made for any directed graph, but we concentrate in particular on the case of boolean recurrent neural networks with convergent/divergent layered structure [1] and recurrence, evolving with a dynamics that includes pruning.

2. Graphs and clique complexes

An *abstract oriented simplicial complex* K [4] is the data of a set K_0 of vertices and sets K_n of lists $\sigma = (x_0, \dots, x_n)$ of elements of K_0 (called *n-simplices*), for $n \geq 1$, with the property that, if $\sigma = (x_0, \dots, x_n)$ belongs to K_n, then any sublist $(x_{i_0}, \dots, x_{i_k})$ of σ belongs to K_k. The sublists of σ are called *faces*.

We consider a finite directed graph $G = (V, E)$ with vertices V and edges E with no self-loops and no double edges, and denote with N the cardinality of V. Associated to G, we can construct its *(oriented) clique complex* $K(G)$, which is the oriented simplicial complex given by $K(G)_0 = V$ and

$$K(G)_n = \{(v_0, \dots, v_n) \colon (v_i, v_j) \in E \text{ for all } i < j\} \quad \text{for } n \geq 1.$$

In other words, an n-simplex contained in $K(G)_n$ is a directed $(n+1)$-clique or a completely connected directed subgraph with $n+1$ vertices.

The clique complex is the basic topological object that allows us to introduce invariants of the graph: the *Euler characteristic* of G is the integer defined by

$$\chi(G) = \sum_{n=0}^{N} (-1)^n \; |K(G)_n|.$$

Let us now consider, for each n, the free abelian group $\mathbb{Z}/2\langle K(G)_n\rangle$ given by the linear combinations of n-simplices with coefficients in the field of two elements $\mathbb{Z}/2$. We can define the *boundary maps* $\partial_n \colon \mathbb{Z}/2\langle K(G)_n\rangle \to \mathbb{Z}/2\langle K(G)_{n-1}\rangle$ which are given by mapping each simplex to the sum of its faces. Then we can define the quantities:

$$\beta_n(G) = \dim(\ker \partial_n) - \dim(\operatorname{Im} \partial_{n+1}),$$

given by the difference of the dimension of the space of the n-simplices whose boundary is zero and the dimension of the space of boundaries of $(n+1)$-simplices. It can be checked that, if we apply a boundary map twice on any linear combination of simplices, we get zero, and so the quantities $\beta_n(G)$ are always non-negative integers. These classically known numbers take the name of *Betti numbers* and, for each n, the n-th Betti number $\beta_n(G)$ corresponds to the dimension of the n-th homology space (with $\mathbb{Z}/2$-coefficients) of the clique complex of G.

The intuitive sense of this construction is to count the "holes" that remain in the graph after we have filled all the directed cliques. In particular, the n-th Betti number is counting the n-dimensional holes. One can also see that β_0 counts the number of connected components of the graph. A classical result in topology shows a connection between the Euler characteristic and the Betti numbers, expressed by the identity: $\chi(G) = \sum_{n=0}^{N}(-1)^n \beta_n(G)$, which gives another way of computing the Euler characteristic.

3. Simulations

We have simulated artificial recurrent neural networks with a layered convergent/divergent connection structure [1]. The networks are composed by 50 layers, each of them with 10 boolean neurons, which can only take values 0 (inactive) or 1 (active) as their status and are all inactive at the beginning. Each neuron in a layer is connected to a fixed proportion of the neurons in the next layer with connections of fixed random weight belonging to one of 4 levels, uniformly distributed between 0 and 1. The neurons in the first layer of the networks are input units, which are activated from outside during the evolution. Moreover, our networks include *recurrence* in their structure, meaning that a small fraction of the neurons are mutually identified in pairs: each pair effectively counts as one unit with the union of the incoming and outgoing connections of the two original neurons.

During the simulation, we activated the input units at a fixed average frequency, and at each step each unit is activated if the sum of the incoming activation from other active cells, weighted by the connection weights, exceeds a fixed threshold.

The network dynamics also implements pruning of the unused connections: if a certain connection does not lead to the activation of its target neuron for a consecutive number of times, its weight is attenuated to the lower level, or the connection is removed from the network, if the weight is already at the lowest level. The pruning serves as a selection of the most significant connections and changes the topology of the network. We have generated a family networks with these features, letting the pruning parameter and the recurrence ratio vary, and computed their dynamical evolution and the evolution of the topological invariants defined above.

4. Results and conclusions

During the simulations, we have computed the Euler characteristic and the Betti numbers and their change during the evolution of the networks, both for the entirety of the nodes in the network and for the sub-network induced by the nodes that are active at each time.

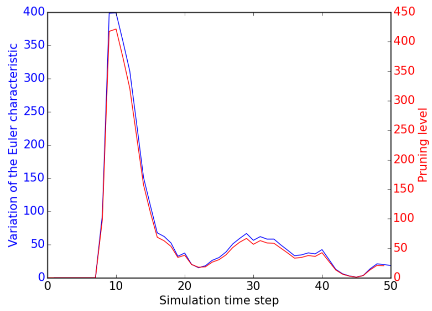

Figure 1: Differences of the Euler characteristic in subsequent steps of the simulation over the time step (in blue) compared to the pruning level, i.e. the number of pruned connections (in red).

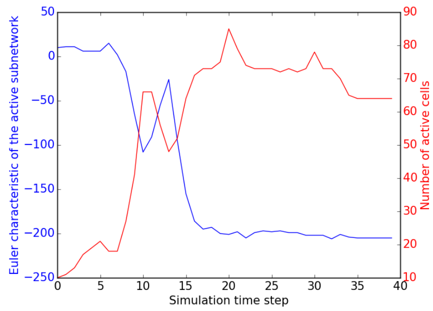

Figure 2: Evolution of the Euler characteristic of the active sub-network (in blue) compared to the number of active units during the network evolution (in red).

Figure 1 and 2 show the evolution of the Euler characteristic respectively for the entirety of the nodes in the network (as an effect of pruning), and for the sub-network of the active nodes. We can see that this invariant can detect changes in the network topology and the patterns of activation of the neurons resulting from the internal dynamics and the external input.

The results of this toy-example are meant to illustrate how Algebraic Topology can provide a solid framework for the study of graphs and a rich variety of useful invariants that can be applied to virtually any problem modelled by a graph, including networks. These invariants are relatively simple to compute for networks, and they can detect and encode their internal connectivity structure and their shape.

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