Dynamics of Evolving Feed-Forward Neural Networks and Their Topological Invariants

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Abstract. The evolution of a simulated feed-forward neural network with recurrent excitatory connections and inhibitory forward connections is studied within the framework of algebraic topology. The dynamics includes pruning and strengthening of the excitatory connections. The invariants that we define are based on the connectivity structure of the underlying graph and its directed clique complex. The computation of this complex and of its Euler characteristic are related with the dynamical evolution of the network. As the network evolves dynamically, its network topology changes because of the pruning and strengthening of the onnections and algebraic topological invariants can be computed at different time steps providing a description of the process. We observe that the initial values of the topological invariant computed on the network before it evolves can predict the intensity of the activity.

Keywords: Graph theory · Network invariant · Directed clique complex · Recurrent neural dynamics · Synfire chain · Synaptic plasticity

1 Introduction

A network is a set of nodes satisfying precise properties of connectedness. This description allows the construction of topological spaces that can be studied with the tools of algebraic topology. Network theory aims to understand and describe the shape and the structure of networks, and the application of the tools developed within the framework of algebraic topology can provide new insights of network properties in several research fields.

The directed clique complex [6,13] is a rigorous way to encode the topological features of a network in the mathematical framework of a simplicial complex, allowing the construction of simple invariants such as the Euler characteristic and the Betti numbers and to make the constructions of persistent homology. These constructions have been applied successfully to the field of data science [4], proving to be a powerful tool to understand the inner structure of a data set by representing it as a sequence of topological spaces, and more recently to neuroscience [6,8,13,14].

In an evolving network, each node is represented by a unit whose activity is necessarily related to a set of precise rules defining the combined activity of the afferent nodes transmitted by the connecting edges. Re-entrant activity occurs in the presence of reciprocal connections between certain nodes. Selected pathways through the network may emerge because of dynamical processes that shape selected activity-dependent connection pruning. Hence, network topology and dynamics combine and play a crucial role in defining the evolution of a network [7]. In a previous study we introduced topological invariants [13] and suggested their application to integrate-and-fire recurrent neural networks with convergent/divergent layered structure [2] with an embedded dynamics of synaptic plasticity. Spontaneous development of synchronous layer activation in a self-organizing recurrent neural network model that combines a number of different plasticity mechanisms has been described [20]. However, the question to what extent the initial network topology can be predictive of the evolved circuit remains to be further investigated.

The current study extends further our previous investigation [13] because global background activity is introduced and inhibitory connections have now been included in the network. The results provide new evidence that the topological invariants presented here offer as a valid descriptor for predicting how a network may evolve under the effect of pruning dynamics. The family of network studied here represents an important step towards the direction of a simulation with more refined biologically-inspired models.

2   Methods

2.1   Graphs, Clique Complexes and Topological Invariants

An *abstract oriented simplicial complex* K [9] is the data of a set K_0 of vertices and sets K_n of lists $\sigma = (x_0, \ldots, x_n)$ of elements of K_0 (called *n-simplices*), for $n \geq 1$, with the property that, if $\sigma = (x_0, \ldots, x_n)$ belongs to K_n, then any sublist $(x_{i_0}, \ldots, x_{i_k})$ of σ belongs to K_k. The sublists of σ are called *faces*.

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

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

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. Notice that an n-simplex is though of as an object of dimension n and consists of $n+1$ vertices.

By definition, a directed clique (or a simplex in our complex) is a fully-connected directed sub-network: this means that the nodes are ordered and there is one source and one sink in the sub-network, and the presence of the directed clique in the network means that the former is connected to the latter in all the possible ways within the sub-network as illustrated by Fig. 1.
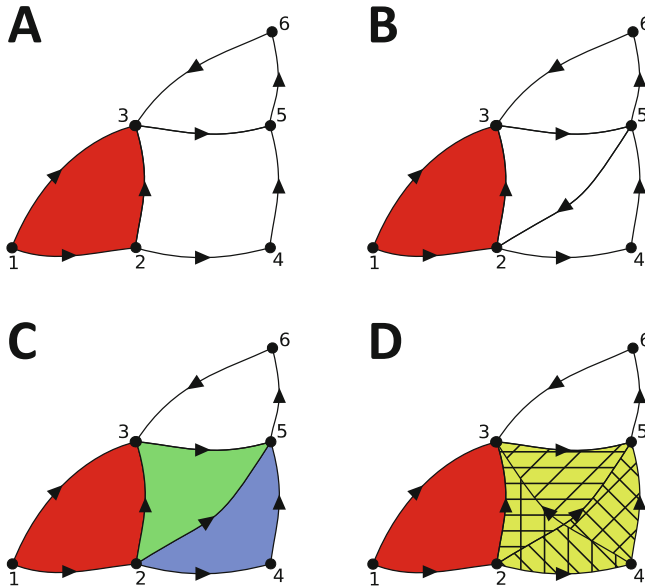
Fig. 1. The directed clique complex. (A) The directed clique complex of the represented graph consists of a 0-simplex for each vertex and a 1-simplex for each edge. There is only one 2-simplex (123). Note that '2453' does not form a 3-simplex because it is not fully connected. '356' does not form a simplex either, because the edges are not oriented correctly. (B) The addition of the edge (52) to the graph in (A) does not contribute to creating any new 2-simplex, because of its orientation. The edges connecting the vertices 2, 3 and 5 (respectively 2, 4 and 5) are oriented cyclically, and therefore they do not follow the conditions of the definition of directed clique complex. (C) By reversing the orientation of the new edge (25), we obtain two new 2-simplices: (235) and (245). Note that we do not have any 3-simplex. (D) We added a new edge (43), thus the subgraph (2435) becomes fully connected and is oriented correctly to be a 3-simplex in the directed clique complex. In addition this construction gives two other 2-simplices: (243) and (435).

The directed clique complex is the basic topological object that allows us to introduce invariants of the graph: the *Euler characteristic* of the directed clique complex $K(G)$ of G is the integer defined by $\chi(K(G)) = \sum_{n=0}^{N}(-1)^n |K(G)_n|$ or in other words the alternating sum of the number of simplices that are present in each dimension. The number of simplices in each dimension (in particular 1- and 2-simplices is also used as invariant of a network.

Notice that the construction of the directed clique complex of a given network G does not involve any choice, and therefore, since the Euler characteristic of a simplicial complex is a well-defined quantities for a simplicial complex [9], our constructions produce quantities that are well-defined for the network G, and we shall refer to them simply as the Euler characteristic of G.

2.2   Network Structure and Dynamics

The artificial recurrent neural networks consist of a finite number of Boolean integrate-and-fire (IF) neurons organized in layers with a convergent/divergent connection structure [2]. The networks are composed by 50 layers, each of them with 10 IF neurons.

The first layer is the layer that receives external stimulations (also referred to as the *input layer*) and all its 10 neurons get activated at the same time at a fixed frequency of 0.1, i.e. every 10 time steps of the history.

Each neuron in a layer is connected to a randomly uniformly distributed number of target neurons f belonging to the next downstream layer. The average distribution of the number of incoming connections is shown in Fig. 2. The networks include *recurrence* in their structure, meaning that a small fraction g of the neurons appears in two different layers. This means that a neuron k that is also identified as neuron l, is characterized by the union of the input connections of neurons k and l, as well as by the union of their respective efferent projections.

We extended the networks constructed in [13] to include inhibition and background activity. A fixed proportion (10 %) of the neurons are inhibitory, the remaining (90 %) are excitatory. The state $S_i(t)$ of a neuron i takes values 0 (inactive) or 1 (active) and all IF neurons are set inactive at the beginning of the simulation. The state $S_i(t)$ is a function of the its activation variable $V_i(t)$, such that $S_i(t) = \mathcal{H}(V_i(t) - 1)$. $\mathcal{H}$ is the Heaviside function, $\mathcal{H}(x) = 0 : x < 0$, $\mathcal{H}(x) = 1 : x \geq 0$, and neurons have a refractory period of one time step after activation. At each time step, the value $V_i(t)$ of the activation variable of the ith neuron is calculated with the formula $V_i(t + 1) = \sum_j S_j(t)w_{ji}(t) + b_i(t)$, where $b_i(t)$ is the background activity, $w_{ji}(t)$ are the weights of the directed connections from any j^{th} neuron projecting to neuron i. The background activity $b_i(t)$ is sampled from a Poisson distribution of parameter $\lambda = 1$ multiplied by a fixed factor of 0.15.

The weights of the excitatory connections have been limited to three values, i.e. $w_1 = 0.1$, $w_2 = 0.2$, and $w_3 = 0.4$. At the beginning of the simulations all connection weights are randomly uniformly distributed among the three possible values. On the opposite, all inhibitory connections are set to $w_4 = -0.2$. The weights of all excitatory connections are updated synchronously at each time step.

The network dynamics implements activity-dependent plasticity of the excitatory connections. Whenever the activation of a connection does not lead to the activation of its target neuron during an interval lasting a time steps, its weight is weakened to the level immediately below the current one. Whenever the weight of an excitatory connection reaches the lowest level without any increase in a time steps, then the connection is removed [10]. The pruning of the connections changes the topology of the network. Similarly, whenever an excitatory connection with a weight w_m is activated at least $m + 1$ consecutive time steps, the connection weight is strengthened to the level immediately higher than the current one. Note though that in the current implementation the inhibitory connections are never pruned and their weights remain constant.
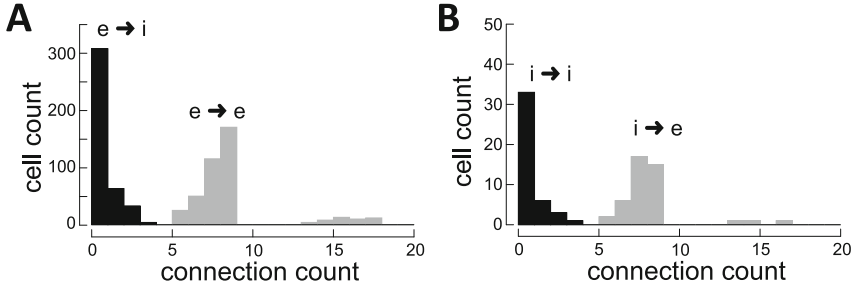
Fig. 2. Cumulative distributions of the efferences within one neural circuit at the begin of the simulation. Network parameters: layer-to-layer downstream connections: 90 %; fraction of recurrent neurons: 10 %; weakening dynamics threshold: 25 steps. (A) excitatory efferent connections to excitatory cells (e→e) and to inhibitory cells (e→i). (B) inhibitory efferent connections to excitatory cells (i→e) and to inhibitory cells (i→i).

Hence, the parameter space of our simulations was defined by three parameters: the number f of layer-to-layer downstream connections in the range 1–10 by steps of 3, the small fraction g of the neurons appearing in two different layers in the range 5–10 % by steps of 5 %, and the interval a of the weakening dynamics of the connections in the range 10–26 by steps of 8.

2.3   Implementation of the Simulations

The simulation software was implemented from scratch in Python. The network evolved with the dynamics explained above and the program computed the directed clique complex at each change of the network topology. The simulation was stopped after 200 time steps, or earlier if the activity died out because of the pruning. For the entire network, the directed clique complex was computed each time the connectivity changed because of pruning. For the sub-network of the active nodes, the computation was carried out at each step of the simulation.

The computed directed clique complexes were used to compute the Euler characteristic both for the complexes representing the entire network and for the sub-complexes of the active nodes. To compute the directed clique complex of a network, we used the algorithm implemented in the `igraph` Python package [5], adapted to find directed cliques, run in parallel on several CPUs using the tool GNU Parallel [16].

3   Results

We considered a directed graph with nodes representing individual neurons and oriented edges representing the connections between the neurons with a weight corresponding to the connection strength. The network topology is based on a simplified model of feed-forward neural network with convergent/divergent layered structure with few embedded recurrent connections and 10 % inhibitory

units at the begin of the simulation. We have computed the Euler characteristic
and its variation during the evolution of such networks in order to detect how
the structure changes as the network evolves. The nodes of the input layer are
activated at regular time intervals.

We observed that the Euler characteristic of the entire network could detect
the pruning activity during the neural network evolution (Fig. 3). In particular,
the step to step variation of the Euler characteristic matched the number of con-
nections pruned over time. The Euler characteristic appears as a good estimator
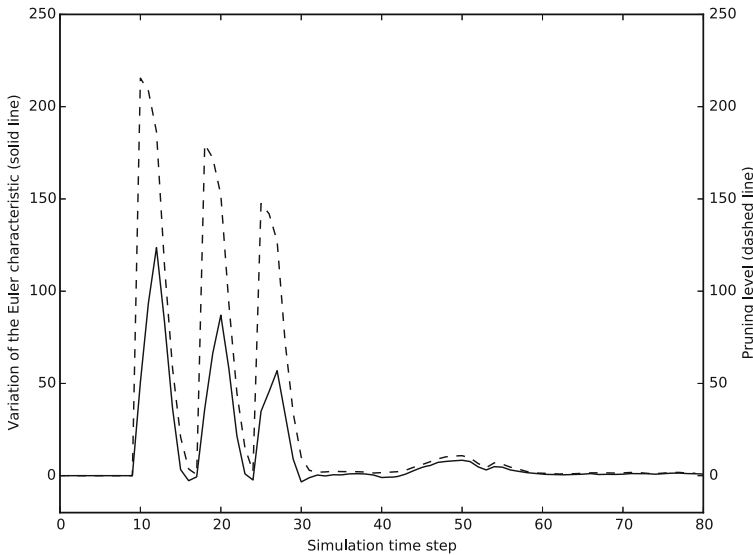of the activity level within the network and of its topological changes.

Fig. 3. The evolution of the Euler characteristic. The plot shows the variation of the
Euler characteristic (averaged across all the networks in the family) over time during
the network evolution (solid line), compared with the plot of the pruning activity
(dashed line). We observe that the Euler characteristic of the direct clique complex of
the entire network detects the changes in the network topology caused by the pruning
activity.

Moreover, despite the more complex dynamics considered in the current sim-
ulation, we found new evidence in favor of the main finding of our previous
study [13]: the type of dynamics undergoing the neural network evolution and
the structure of the directed clique complex of that network at the very begin-
ning of the simulation (i.e. before the occurrence of connection pruning) were
correlated. In particular, the average number of active units during the simula-
tion was correlated to the number of simplices, in the directed clique complex,
of dimension two (Pearson correlation coefficient $r_{(190)} = 0.50$, $p < 0.001$) and
dimension three ($r_{(190)} = 0.50$, $p < 0.001$).

Even in presence of different network dynamics, the initial connectivity structure of the network contains a algebraic-topological information that can be used to predict the type of evolution that the network is going to have. The rationale for it being correlated with the number of high (2 and 3) dimensional simplices is that directed cliques are fully connected sub-networks, i.e. sub-networks with an initial and a final node that are connected in the highest possible number of ways, and thus they contribute to the propagation of the activation.

4   Discussion

Network topology and dynamics are closely related: the convergent/divergent networks with neurons organised in layers in a feed-forward structure, which we considered here, are closely associated with synfire chains [1,2]. These networks are characterized by a highly correlated activity of the neurons within each later, propagated from a layer to the next one, which is the kind of behaviour that we observed in our simulations. The temporal patterns of activation displayed by synfire chains are of central importance in the transmission of neural information [11], and experimental results in electrophysiology show the emergence of precise patterns of activation [15,17], associated with neural functions such as sensory encoding and cognitive responses.

The networks considered here are a version of synfire chains, with the simplification that the chain structure forms the entirety of the network: for this reason we do not investigate the important problem of the emergence of synfire chains embedded in bigger networks. This question has been investigated in relation with several network features, as a function of network topology and plasticity rules [18–20]. Our simulations show that the excitatory-inhibitory and the background noise are central elements in the maintenance of a steady and irregular activity level [3,12]: the maintenance of a non-saturated activity level for the duration of the simulations is necessary in order to correlate the average activity of the networks with the topological invariants that we have presented here. The addition of inhibitory neurons and background activity with respect to our previous study [13] gave richer and more complicated dynamics, and yet we found that our tools can shed light on the links between network topology and pruning dynamics. The algebro-topological framework of analysis presented here appears as a very promising technique and deserves further study in order to investigate the deeper relations between temporal activation patterns and network topology in biologically inspired networks.

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