The topology of the directed clique complex as a network invariant

Paolo Masulli and Alessandro E. P. Villa

Presented by Shreeya Behera

March 22, 2022

Layout

- Motivations.

Layout

- Motivations.
- Definitions of directed clique complex.

Layout

- Motivations.
- Definitions of directed clique complex.
- Boolean recurrent artificial neural network.

Layout

- Motivations.
- Definitions of directed clique complex.
- Boolean recurrent artificial neural network.
    - Model and Method
    - Results

Layout

- Motivations.
- Definitions of directed clique complex.
- Boolean recurrent artificial neural network.
  - Model and Method
  - Results
- Network filtrations.

Layout

- Motivations.
- Definitions of directed clique complex.
- Boolean recurrent artificial neural network.
  - Model and Method
  - Results
- Network filtrations.
  - Model and Method
  - Results

Layout

- Motivations.
- Definitions of directed clique complex.
- Boolean recurrent artificial neural network.
  - Model and Method
  - Results
- Network filtrations.
  - Model and Method
  - Results
- Conclusions.

Motivations

- The directed clique complex helps us to encode the topological features of a network in the mathematical framework of a simplicial complex.

Motivations

- The directed clique complex helps us to encode the topological features of a network in the mathematical framework of a simplicial complex.
- This allows the construction of a class of invariants such as the Euler characteristic and the Betti numbers.

Motivations

- The directed clique complex helps us to encode the topological features of a network in the mathematical framework of a simplicial complex.
- This allows the construction of a class of invariants such as the Euler characteristic and the Betti numbers.
- Using Euler characteristics we can predicts how the network is going to evolve under the effect of the pruning dynamics.

Motivations

- The directed clique complex helps us to encode the topological features of a network in the mathematical framework of a simplicial complex.
- This allows the construction of a class of invariants such as the Euler characteristic and the Betti numbers.
- Using Euler characteristics we can predicts how the network is going to evolve under the effect of the pruning dynamics.
- The Euler characteristic computed on a sequence of networks generated by filtrating its nodes by in- and out-degrees is helpful for a network classification.

Graphs and clique complexes

An abstract oriented simplicial complex K 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,

Graphs and clique complexes

An abstract oriented simplicial complex K 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.

Graphs and clique complexes

An abstract oriented simplicial complex K 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 weighted simple graph $G = (V, E)$ with vertex set V and edge set E, with $|V| = N$.

We consider a finite directed weighted simple graph $G = (V, E)$ with vertex set V and edge set E, with $|V| = N$.

Using G, (directed) clique complex $K(G)$ is constructed, which is the directed simplicial complex given by $K(G)_0 = V$ and $K(G)_n = \{(v_0, \ldots, v_n) : (v_i, v_j) \in E \text{ for all } i < j\} \quad \text{for } n \geq 1.$

We consider a finite directed weighted simple graph $G = (V, E)$ with vertex set V and edge set E, with $|V| = N$.

Using G, (directed) clique complex $K(G)$ is constructed, which is the directed simplicial complex given by $K(G)_0 = V$ and $K(G)_n = \{(v_0, \ldots, v_n) : (v_i, v_j) \in E \text{ for all } i < j\} \quad \text{for } n \geq 1.$

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

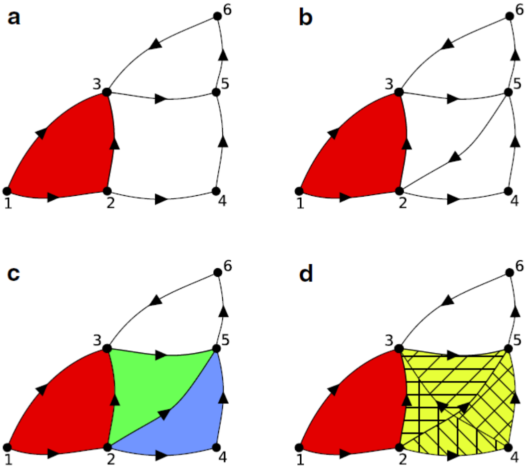


Figure: The directed clique complex

The topological invariants

The Euler characteristic of the directed clique complex $K(G)$ of G is the integer defined by

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

Recall

The boundary maps $\partial_n : \mathbf{Z}/2\langle K(G)_n\rangle \to \mathbf{Z}/2\langle K(G)_{n-1}\rangle$ which are given by mapping each simplex to the sum of its faces. Then we can define the quantities:

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

Connection between the Euler characteristic and the Betti numbers

$$\chi(K(G)) = \sum_{n=0}^{N} (-1)^n \beta_n(K(G))$$

Boolean recurrent artificial neural networks

- The networks are composed by 50 layers, each of them with 10 Boolean neurons.

Boolean recurrent artificial neural networks

- The networks are composed by 50 layers, each of them with 10 Boolean neurons.
- The first layer is the input layer and all its 10 neurons get activated at the same time at a fixed frequency.

Boolean recurrent artificial neural networks

- The networks are composed by 50 layers, each of them with 10 Boolean neurons.
- The first layer is the input layer and all its 10 neurons get activated at the same time at a fixed frequency.
- Each neuron in a layer is connected to a randomly uniformly distributed number of target neurons f belonging to the next downstream layer.

- The state $S_i(t)$ of a neuron i take values 0 or 1 and all Boolean neurons are set inactive at the beginning of the simulation.

- The state $S_i(t)$ of a neuron i take values 0 or 1 and all Boolean neurons are set inactive at the beginning of the simulation.
- The state $S_i(t)$ is a function of the its activation variable $V_i(t)$ and a threshold θ, such that $S_i(t) = \mathcal{H}\left(V_i(t) - \theta\right)$.

- The state $S_i(t)$ of a neuron i take values 0 or 1 and all Boolean neurons are set inactive at the beginning of the simulation.
- The state $S_i(t)$ is a function of the its activation variable $V_i(t)$ and a threshold θ, such that $S_i(t) = \mathcal{H}\left(V_i(t) - \theta\right)$.
- $\mathcal{H}$ is the Heaviside function, $\mathcal{H}(x) = 0 : x < 0, \mathcal{H}(x) = 1 : x \geq 0$.

- The state $S_i(t)$ of a neuron i take values 0 or 1 and all Boolean neurons are set inactive at the beginning of the simulation.
- The state $S_i(t)$ is a function of the its activation variable $V_i(t)$ and a threshold θ, such that $S_i(t) = \mathcal{H}\left(V_i(t) - \theta\right)$.
- $\mathcal{H}$ is the Heaviside function, $\mathcal{H}(x) = 0 : x < 0, \mathcal{H}(x) = 1 : x \geq 0$.
- At each time step, the value $V_i(t)$ of the activation variable of the i th neuron is calculated such that $V_i(t+1) = \sum_j S_j(t) w_{ji}(t)$, where $w_{ji}(t)$ are the weights.

- The state $S_i(t)$ of a neuron i take values 0 or 1 and all Boolean neurons are set inactive at the beginning of the simulation.
- The state $S_i(t)$ is a function of the its activation variable $V_i(t)$ and a threshold θ, such that $S_i(t) = \mathcal{H}\left(V_i(t) - \theta\right)$.
- $\mathcal{H}$ is the Heaviside function, $\mathcal{H}(x) = 0 : x < 0, \mathcal{H}(x) = 1 : x \geq 0$.
- At each time step, the value $V_i(t)$ of the activation variable of the i th neuron is calculated such that $V_i(t+1) = \sum_j S_j(t) w_{ji}(t)$, where $w_{ji}(t)$ are the weights.
- The connection weights can only take four values, i.e. $w_1 = 0.1, w_2 = 0.2, w_3 = 0.4, w_4 = 0.8$.

- Whenever the activation of a connection does not lead to the activation of its target neuron during a certain number of steps, its weight is weakened to the level immediately lower than the current one.

- Whenever the activation of a connection does not lead to the activation of its target neuron during a certain number of steps, its weight is weakened to the level immediately lower than the current one.
- Whenever the weight of a connection reaches the lowest level, the connection is removed from the network.

- Whenever the activation of a connection does not lead to the activation of its target neuron during a certain number of steps, its weight is weakened to the level immediately lower than the current one.
- Whenever the weight of a connection reaches the lowest level, the connection is removed from the network.
- The pruning of the connections provokes the selection of the most significant ones and changes the topology of the network.

Results of dynamics of artificial neural networks

- The directed clique complex is computed using the dynamic we saw.

Results of dynamics of artificial neural networks

- The directed clique complex is computed using the dynamic we saw.
- The Euler characteristic and its variation during the evolution of such networks is calculated.

Results of dynamics of artificial neural networks

- The directed clique complex is computed using the dynamic we saw.
- The Euler characteristic and its variation during the evolution of such networks is calculated.
- It is calculated 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 step.

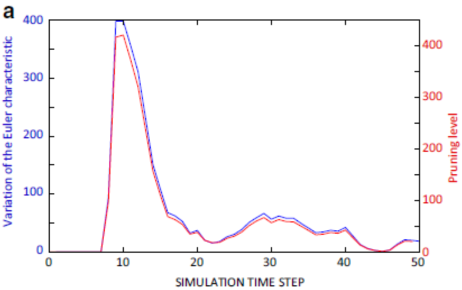


Figure: **a** Euler characteristic in subsequent steps of the simulation over time (blue curve) compared to the pruning level (red curve), i.e. the number of pruned connections.

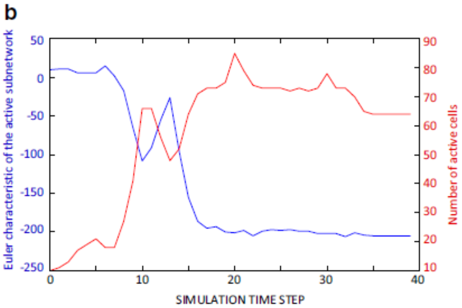


Figure: **b** Evolution of the Euler characteristic of the active sub-network (blue curve) compared to the number of active units during the network evolution (red curve). Notice that the two curves are negatively correlated.

Network filtrations

Many essential topological features of a network are determined by the distribution of edges over its graph.

Network filtrations

Many essential topological features of a network are determined by the distribution of edges over its graph.

Different types of distributions result in different types of networks.

Network filtrations

Many essential topological features of a network are determined by the distribution of edges over its graph.

Different types of distributions result in different types of networks.

In this article, the following three types of graph were consider:

Network filtrations

Many essential topological features of a network are determined by the distribution of edges over its graph.

Different types of distributions result in different types of networks.

In this article, the following three types of graph were consider:

- Random Networks (Erdos-Renyi Model)

Network filtrations

Many essential topological features of a network are determined by the distribution of edges over its graph.

Different types of distributions result in different types of networks.

In this article, the following three types of graph were consider:

- Random Networks (Erdos-Renyi Model)
- Small-World Networks (Watts and Strogatz Model)

Network filtrations

Many essential topological features of a network are determined by the distribution of edges over its graph.

Different types of distributions result in different types of networks.

In this article, the following three types of graph were consider:

- Random Networks (Erdos-Renyi Model)
- Small-World Networks (Watts and Strogatz Model)
- Scale-Free Networks (Barabasi Albert Model)

Random Networks (Erdos-Renyi Model)

- A random network is the one in which there is a certain probability for a link between any two nodes in the network.

Random Networks (Erdos-Renyi Model)

- A random network is the one in which there is a certain probability for a link between any two nodes in the network.
- Erdos-Renyi Model (ER) Model
  - The probability for a link between any two nodes is the same.

Random Networks (Erdos-Renyi Model)

- A random network is the one in which there is a certain probability for a link between any two nodes in the network.
- Erdos-Renyi Model (ER) Model
  - The probability for a link between any two nodes is the same.
  - We represent the model as $G(N, p)$where N is the number of nodes and p is the probability for a link between any two nodes.

Small-World Networks (Watts and Strogatz Model)

- Watts and Strogatz (WS) Model
  - Let N be the number of nodes and K (assumed to be even) be the mean degree.

Small-World Networks (Watts and Strogatz Model)

- Watts and Strogatz (WS) Model
  - Let N be the number of nodes and K (assumed to be even) be the mean degree.
  - Initially, let there be a regular ring lattice of N nodes, with K neighbors (K/2 neighbors on each side).

Small-World Networks (Watts and Strogatz Model)

- Watts and Strogatz (WS) Model
  - Let N be the number of nodes and K (assumed to be even) be the mean degree.
  - Initially, let there be a regular ring lattice of N nodes, with K neighbors (K/2 neighbors on each side).
  - For every node $n_i = n_0, n_1, \ldots, n_{N-1}$, rewire the edge (n_i, n_j), where $i < j$, with some probability p, i.e.

Small-World Networks (Watts and Strogatz Model)

- Watts and Strogatz (WS) Model
  - Let N be the number of nodes and K (assumed to be even) be the mean degree.
  - Initially, let there be a regular ring lattice of N nodes, with K neighbors (K/2 neighbors on each side).
  - For every node $n_i = n_0, n_1, \ldots, n_{N-1}$, rewire the edge (n_i, n_j), where $i < j$, with some probability p, i.e. replacing (n_i, n_j) with (n_i, n_k) where n_k is chosen uniform randomly among all possible nodes that avoid self-looping and link duplication.

Scale-Free Networks (Barabasi Albert Model)

- The model is defined as follows:

Scale-Free Networks (Barabasi Albert Model)

- The model is defined as follows:
  - We start with n nodes, the links between which are chosen arbitrarily, as long as each node has at least one link.

Scale-Free Networks (Barabasi Albert Model)

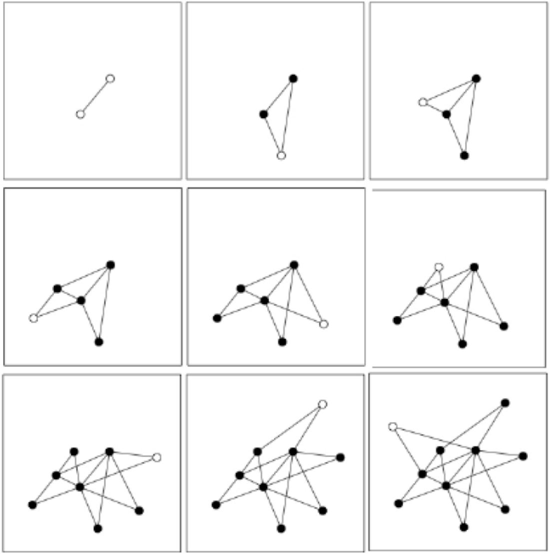
- The model is defined as follows:
  - We start with n nodes, the links between which are chosen arbitrarily, as long as each node has at least one link.
  - At each time step, we add a new node with $m\,(\leq n)$ links that connect the new node to m nodes already in the network.

Scale-Free Networks (Barabasi Albert Model)

- The model is defined as follows:
  - We start with n nodes, the links between which are chosen arbitrarily, as long as each node has at least one link.
  - At each time step, we add a new node with $m\,(\leq n)$ links that connect the new node to m nodes already in the network.
  - The probability that one of the links of the new node connects to node i depends on the degree k_i of node i as:

Scale-Free Networks (Barabasi Albert Model)

- The model is defined as follows:
  - We start with n nodes, the links between which are chosen arbitrarily, as long as each node has at least one link.
  - At each time step, we add a new node with $m\,(\leq n)$ links that connect the new node to m nodes already in the network.
  - The probability that one of the links of the new node connects to node i depends on the degree k_i of node i as: a node with larger degree has good chances of getting connected to even more nodes



BA Model Example (m = 2)

Source: Figure 5.4
Barabasi

Network degree invariant

Given a directed network G, we define two filtrations by sub-networks using the in- and out-degree of nodes.

Network degree invariant

Given a directed network G, we define two filtrations by sub-networks using the in- and out-degree of nodes.

Let $ODF(G)$ be the out-degree filtration of G:
the i-th network $ODF(G)_i$ in this filtration is the sub-network of G induced by the vertices having out-degree at least i and all the target nodes of their outgoing connections.

Network degree invariant

Given a directed network G, we define two filtrations by sub-networks using the in- and out-degree of nodes.

Let $ODF(G)$ be the out-degree filtration of G:
the *i-th* network $ODF(G)_i$ in this filtration is the sub-network of G induced by the vertices having out-degree at least i and all the target nodes of their outgoing connections.

Similarly, we can define in-degree filtration of G, $IDF(G)$.

Method: Network filtrations and invariants

- The Euler characteristic on a sequence of sub-networks defined by the in- and out-degrees of the vertices is computed.

Method: Network filtrations and invariants

- The Euler characteristic on a sequence of sub-networks defined by the in- and out-degrees of the vertices is computed.
- The sequences of the Euler characteristic of the in-degree and the out-degree filtrations are plotted as a function of the normalized minimum degree of vertices.

Method: Network filtrations and invariants

- The Euler characteristic on a sequence of sub-networks defined by the in- and out-degrees of the vertices is computed.
- The sequences of the Euler characteristic of the in-degree and the out-degree filtrations are plotted as a function of the normalized minimum degree of vertices.
- This normalization is necessary to compare networks of different sizes at each filtration level posing the maximum degree of the vertices in the network to 1.

Method: Network filtrations and invariants

- The Euler characteristic on a sequence of sub-networks defined by the in- and out-degrees of the vertices is computed.
- The sequences of the Euler characteristic of the in-degree and the out-degree filtrations are plotted as a function of the normalized minimum degree of vertices.
- This normalization is necessary to compare networks of different sizes at each filtration level posing the maximum degree of the vertices in the network to 1.
- Each network type was simulated 50 times using different random seeds.

Results

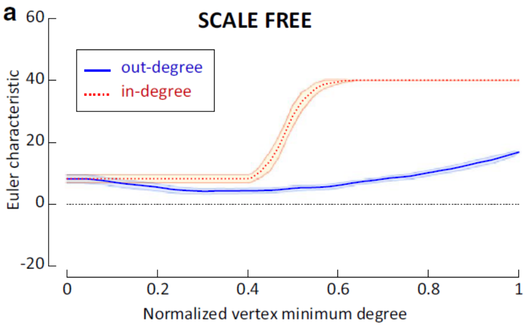


Figure: Plot of the degree-filtered Euler characteristic generated with $n = 40$ nodes, and $m = 10$.

The values of the Euler characteristic of the in-degree filtration is always larger than the curve of the out-degree filtration.

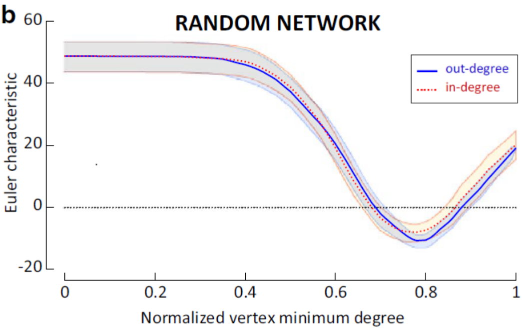


Figure: Plot of the degree-filtered Euler characteristic generated with $n = 40$ nodes, and $p = 0.2$.

The curves of in- and out-degrees overlap at all levels of the filtration.

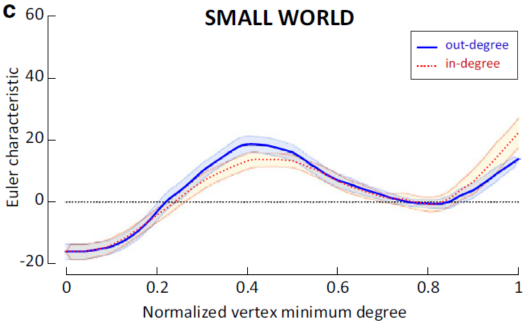


Figure: Plot of the degree-filtered Euler characteristic generated with $n = 40$ nodes, $k = 20$, and $p = 0.4$.

Both curves of in- and out-degrees start from the minimal value of the Euler characteristic with the least vertex minimum degree, followed by a non monotonic increase and a tendency of overlap between the two curves

Conclusions

- Simple invariants such as the Euler characteristic can detect the changes in the network topology.
- The results shown here are a contribution to the application of algebraic topology to the study of more complex networks and their dynamics.

References

1. Masulli P., Villa A.E.P. The topology of the directed clique complex as a network invariant. *SpringerPlus 5, 388 (2016).* https://doi.org/10.1186/s40064-016-2022-y
2. Reimann, M. W. et al. Cliques of neurons bound into cavitiesprovide a missing link between structure and function, *Frontiersin Comp. Neuro. 11, 48 (2017).* https://doi.org/10.3389/fncom.2017.00048
3. Network Science by Albert-László Barabási, *Cambridge University Press* (2016).isbn=9781107076266 https://books.google.com/books?id=iLtGDQAAQBAJ