Higher-order networks

An introduction to simplicial complexes
Lesson I

Franqui Chair Lessons

18-19 April 2023

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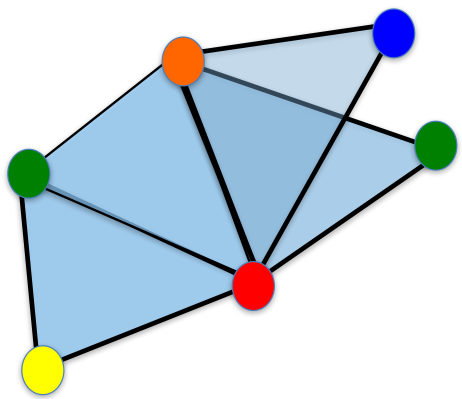
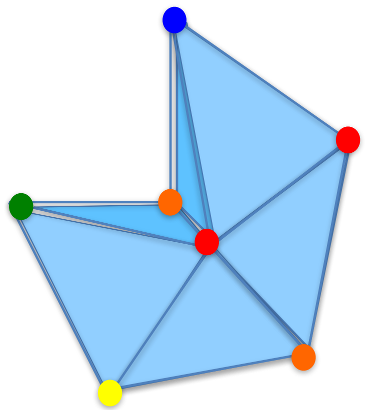
Higher-order networks

Higher-order networks are characterising the interactions between two ore more nodes and are formed by nodes, links, triangles, tetrahedra etc.



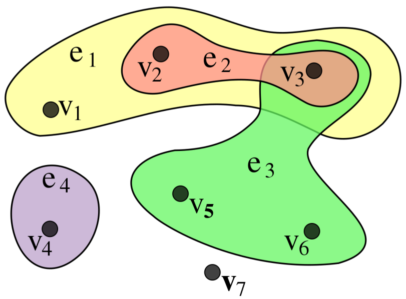
d=2 simplicial complex



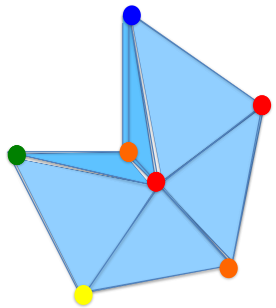
d=3 simplicial complex

Higher-order networks

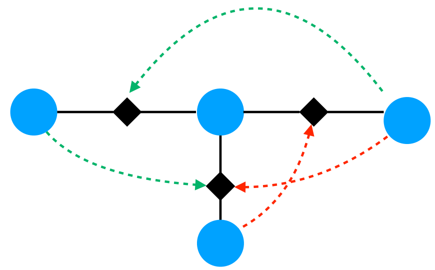
Higher-order networks are characterising the interactions between two or more nodes



Hypergraph

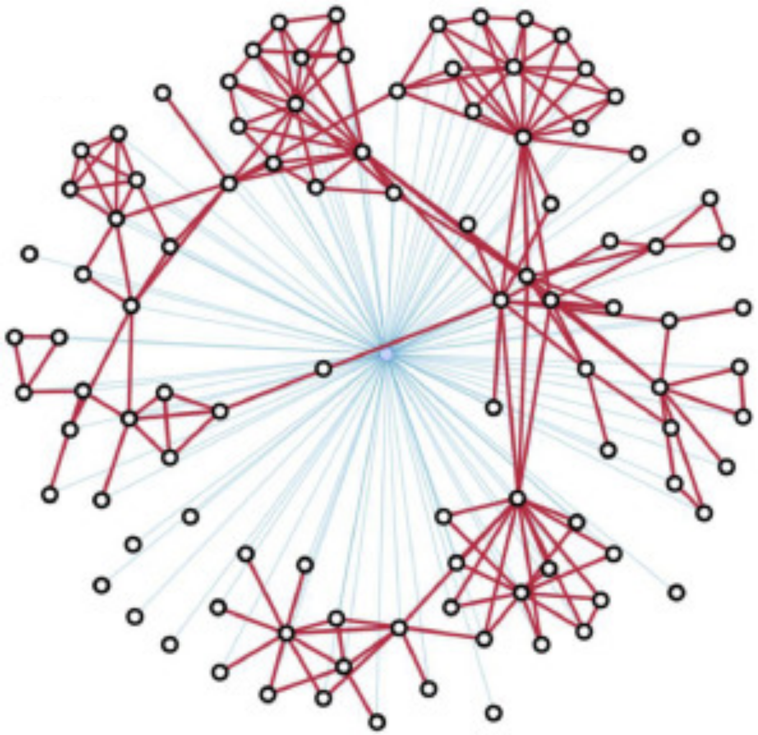


Simplicial complex



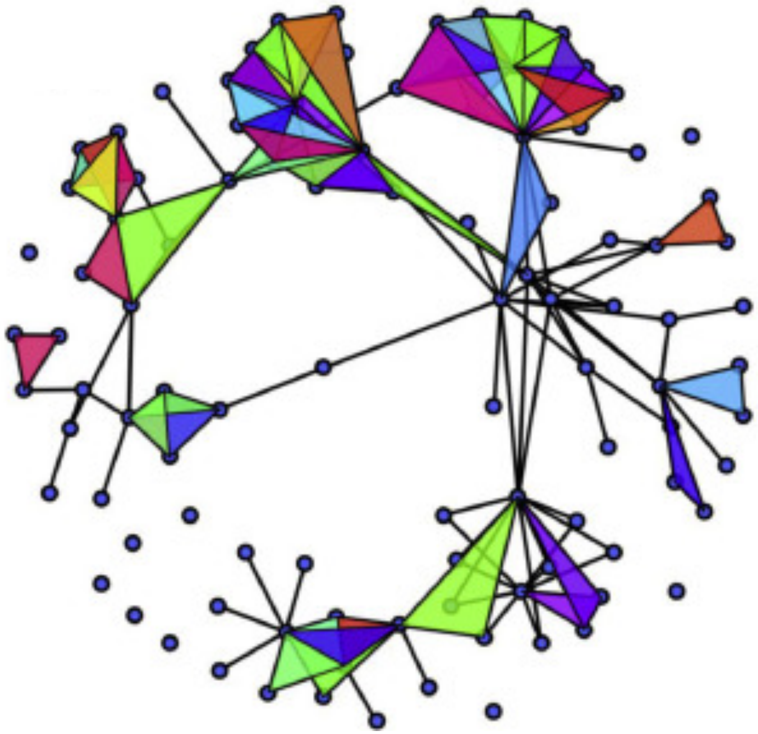
Network with triadic interactions

Networks



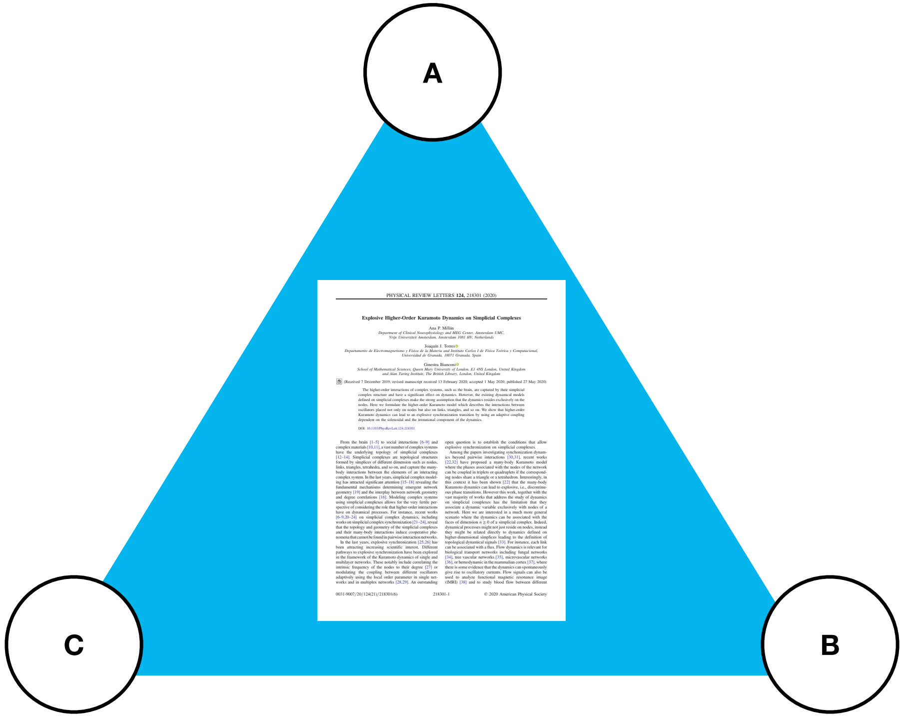
Simple network

Higher-order networks



Simplicial complex

Higher order network



PHYSICAL REVIEW LETTERS **124,** 218301 (2020)

Explosive Higher-Order Kuramoto Dynamics on Simplicial Complexes

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The higher-order interactions of complex systems, such as the brain, are captured by their simplicial complex structure and have a significant effect on dynamics. However, the existing dynamical models defined on simplicial complexes make the strong assumption that the dynamics resides exclusively on the nodes. Here we formulate the higher-order Kuramoto model which describes the interactions between oscillators placed not only on nodes but also on links, triangles, and so on. We show that higher-order Kuramoto dynamics can lead to an explosive synchronization transition by using an adaptive coupling dependent on the solenoidal and the irrotational component of the dynamics.

DOI: 10.1103/PhysRevLett.124.218301

From the brain [1–5] to social interactions [6–9] and complex materials [10,11], a vast number of complex systems have the underlying topology of simplicial complexes [12–14]. Simplicial complexes are topological structures formed by simplices of different dimension such as nodes, links, triangles, tetrahedra, and so on, and capture the many-body interactions between the elements of an interacting complex system. In the last years, simplicial complex modeling has attracted significant attention [15–18] revealing the fundamental mechanisms determining emergent network geometry [19] and the interplay between network geometry and degree correlations [16]. Modeling complex systems using simplicial complexes allows for the very fertile perspective of considering the role that higher-order interactions have on dynamical processes. For instance, recent works [6–9,20–24] on simplicial complex dynamics, including works on simplicial complex synchronization [21–24], reveal that the topology and geometry of the simplicial complexes and their many-body interactions induce cooperative phenomena that cannot be found in pairwise interaction networks.

In the last years, explosive synchronization [25,26] has been attracting increasing scientific interest. Different pathways to explosive synchronization have been explored in the framework of the Kuramoto dynamics of single and multilayer networks. These notably include correlating the intrinsic frequency of the nodes to their degree [27] or modulating the coupling between different oscillators adaptively using the local order parameter in single networks and in multiplex networks [28,29]. An outstanding open question is to establish the conditions that allow explosive synchronization on simplicial complexes.

Among the papers investigating synchonization dynamics beyond pairwise interactions [30,31], recent works [22,32] have proposed a many-body Kuramoto model where the phases associated with the nodes of the network can be coupled in triplets or quadruplets if the corresponding nodes share a triangle or a tetrahedron. Interestingly, in this context it has been shown [22] that the many-body Kuramoto dynamics can lead to explosive, i.e., discontinuous phase transitions. However this work, together with the vast majority of works that address the study of dynamics on simplicial complexes has the limitation that they associate a dynamic variable exclusively with nodes of a network. Here we are interested in a much more general scenario where the dynamics can be associated with the faces of dimension $n \geq 0$ of a simplicial complex. Indeed, dynamical processes might not just reside on nodes, instead they might be related directly to dynamics defined on higher-dimensional simplices leading to the definition of topological dynamical signals [33]. For instance, each link can be associated with a flux. Flow dynamics is relevant for biological transport networks including fungal networks [34], tree vascular networks [35], microvascular networks [36], or hemodynamic in the mammalian cortex [37], where there is some evidence that the dynamics can spontaneously give rise to oscillatory currents. Flow signals can also be used to analyze functional magnetic resonance image (fMRI) [38] and to study blood flow between different

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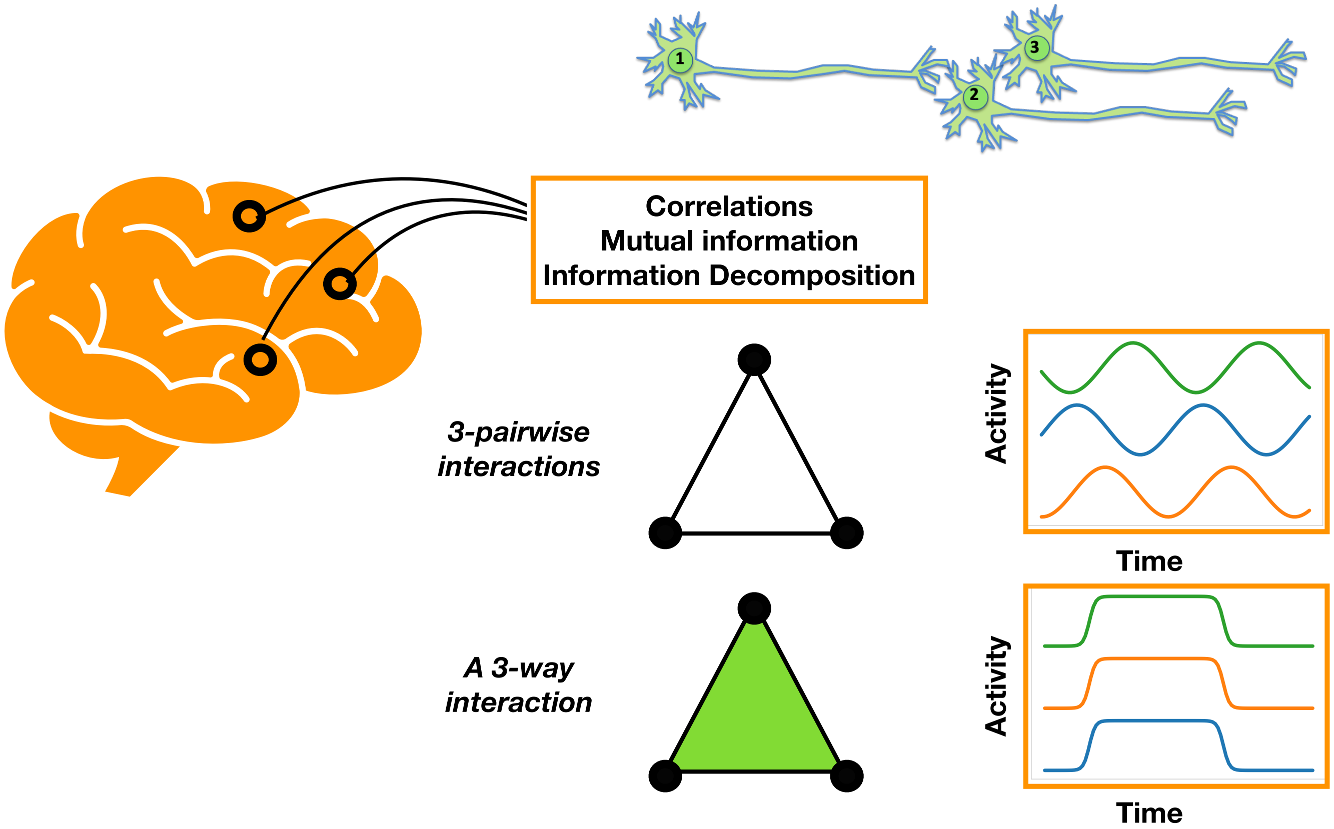
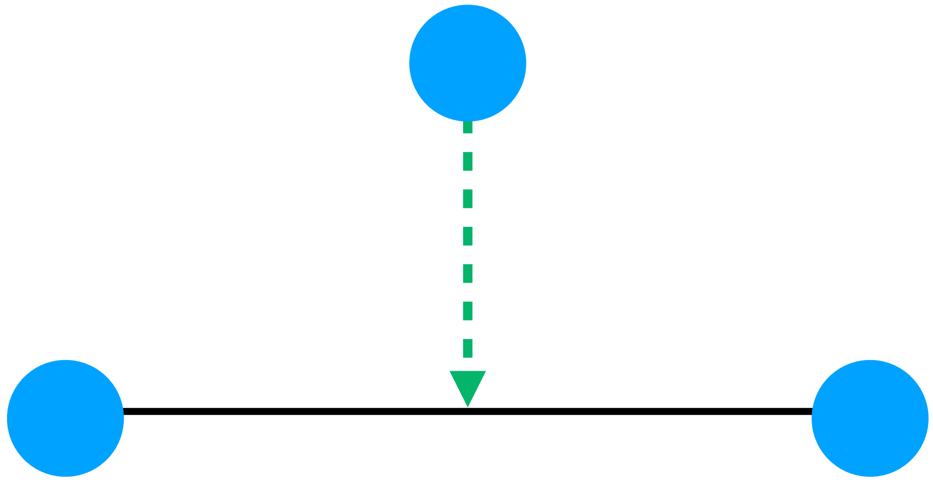
Collaboration network

Higher-order network

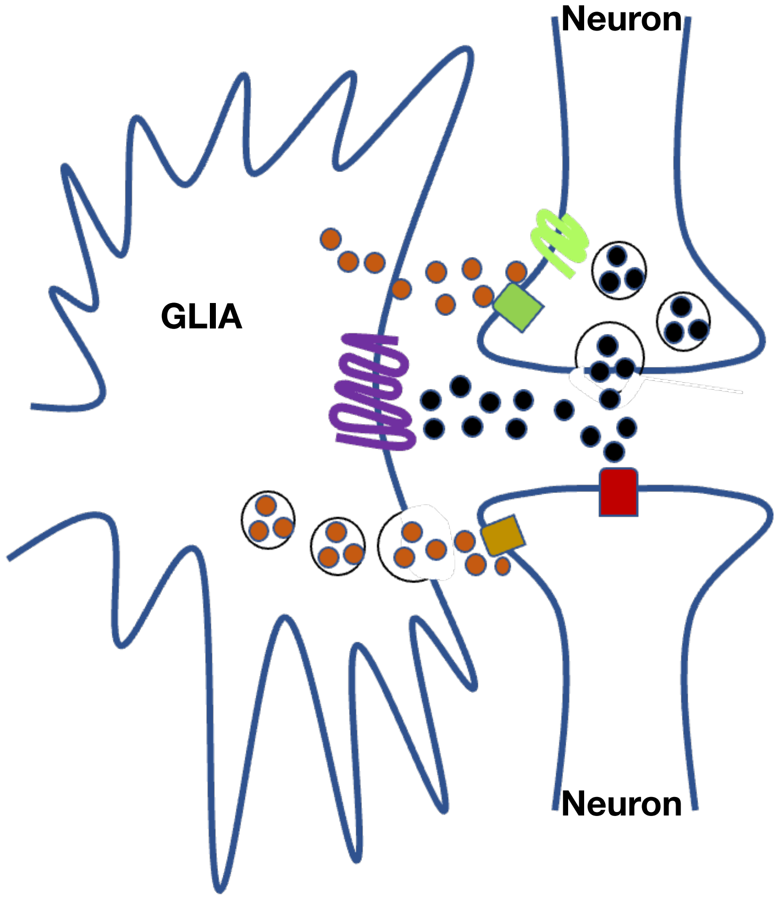


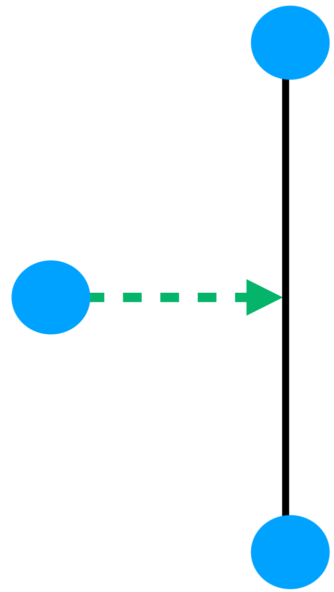
Triadic interactions



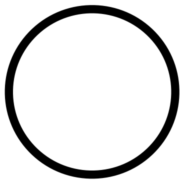
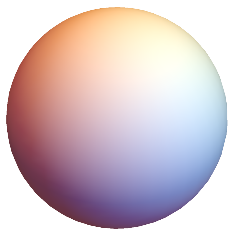
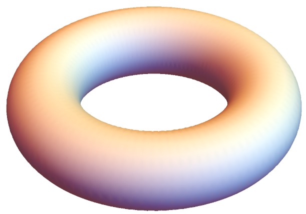
A triadic interaction occurs when a node affects the interaction between other two nodes

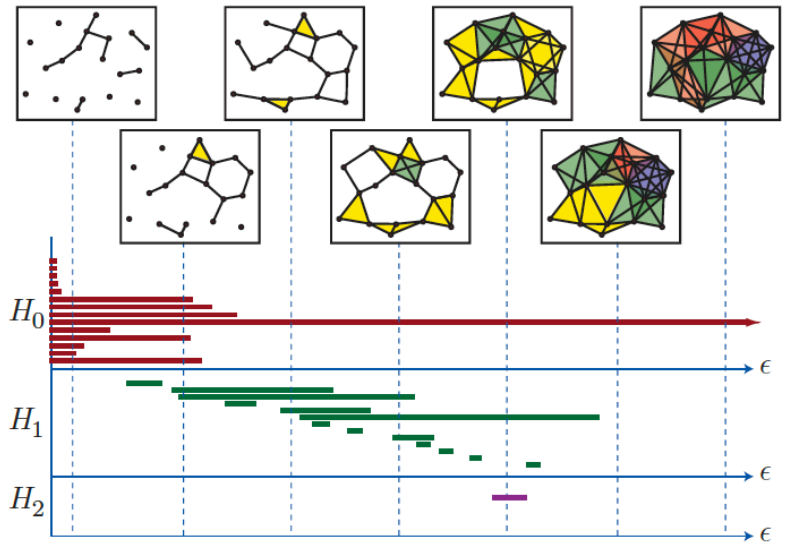
Triadic interactions between neurons and glia





What Is Topology?

Point	Circle	Sphere	Torus
			
$\beta_0 = 1$	$\beta_0 = 1$	$\beta_0 = 1$	$\beta_0 = 1$
$\beta_1 = 0$	$\beta_1 = 1$	$\beta_1 = 0$	$\beta_1 = 2$
$\beta_2 = 0$	$\beta_2 = 0$	$\beta_2 = 1$	$\beta_2 = 1$

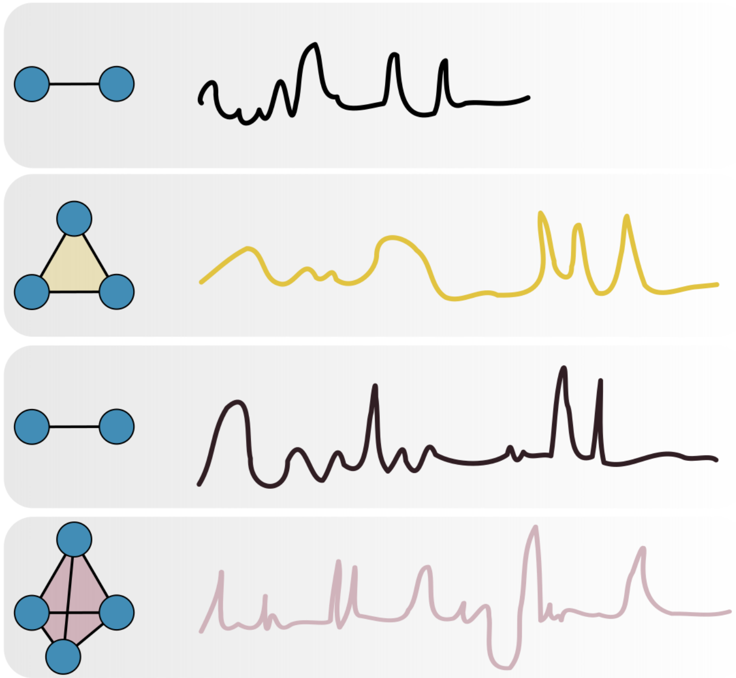


Ghrist 2008

Topological signals

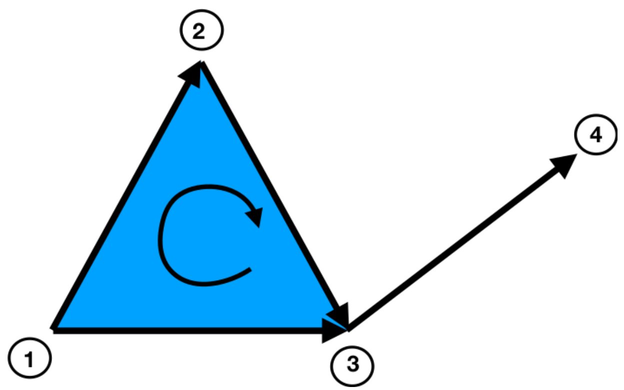
Topological signals are not only defined on nodes but also on links, triangles and higher-order simplices

- Synaptic signal
- Edge signals in the brain
- Citations in a collaboration network
- Speed of wind at given locations
- Currents at given locations in the ocean
- Fluxes in biological transportation networks



Battiston et al. Nature Physics 2021

Boundary Operators



Boundary operators

$$\mathbf{B}_{[1]} = \begin{array}{c|cccc} & [1,2] & [1,3] & [2,3] & [3,4] \\ \hline [1] & -1 & -1 & 0 & 0 \\ [2] & 1 & 0 & -1 & 0 \\ [3] & 0 & 1 & 1 & -1 \\ [4] & 0 & 0 & 0 & 1 \end{array}, \qquad \mathbf{B}_{[2]} = \begin{array}{c|c} & [1,2,3] \\ \hline [1,2] & 1 \\ [1,3] & -1 \\ [2,3] & 1 \\ [3,4] & 0 \end{array}.$$

$\mathbf{B}_{[1]}$ **Discrete divergence**

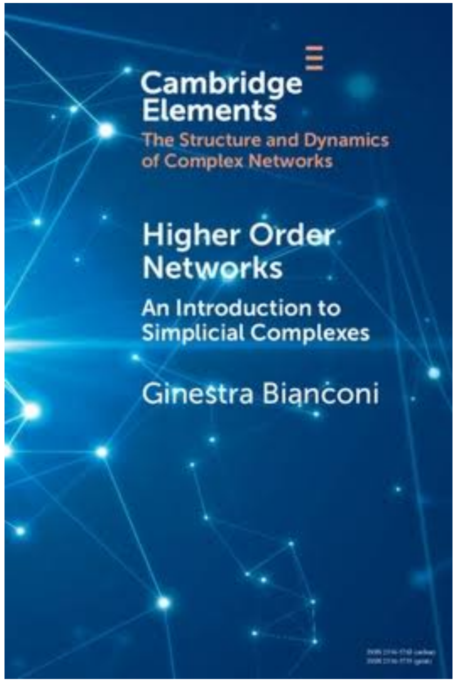
$\mathbf{B}_{[1]}^\top$ **Discrete gradient**

$\mathbf{B}_{[2]}^\top$ **Discrete Curl**

The boundary of the boundary is null

$$\mathbf{B}_{[m-1]}\mathbf{B}_{[m]} = \mathbf{0}, \quad \mathbf{B}_{[m]}^\top\mathbf{B}_{[m-1]}^\top = \mathbf{0}$$

Higher-order networks



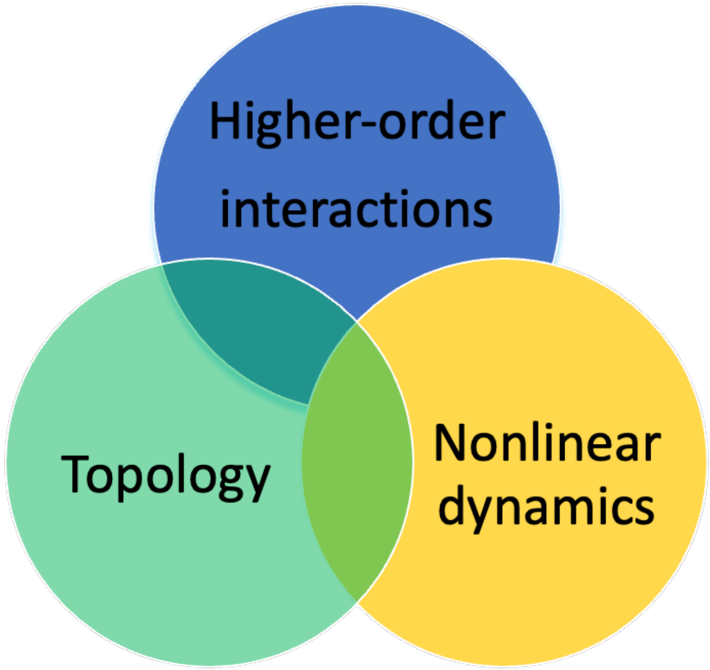
New book
by Cambridge University Press

Providing a general view of the interplay between topology and dynamics

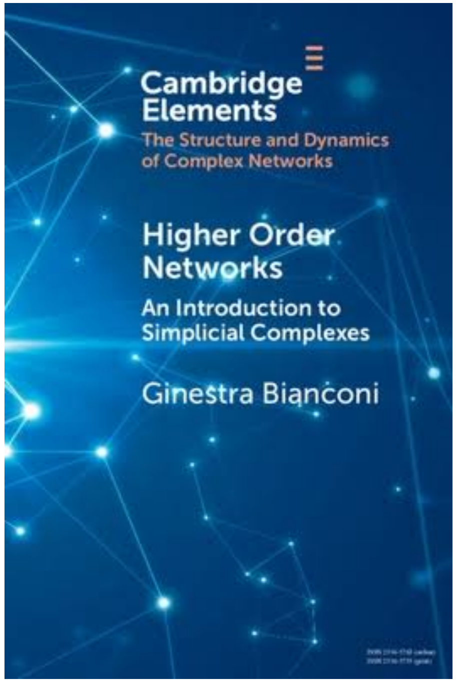
Can we learn the dynamics from the complex system topology?

Can we learn the topology from the complex system dynamics?

Complexity challenge



Higher-order networks



New book
by Cambridge University Press!!

Providing a general view of the interplay between topology and dynamics

nature physics

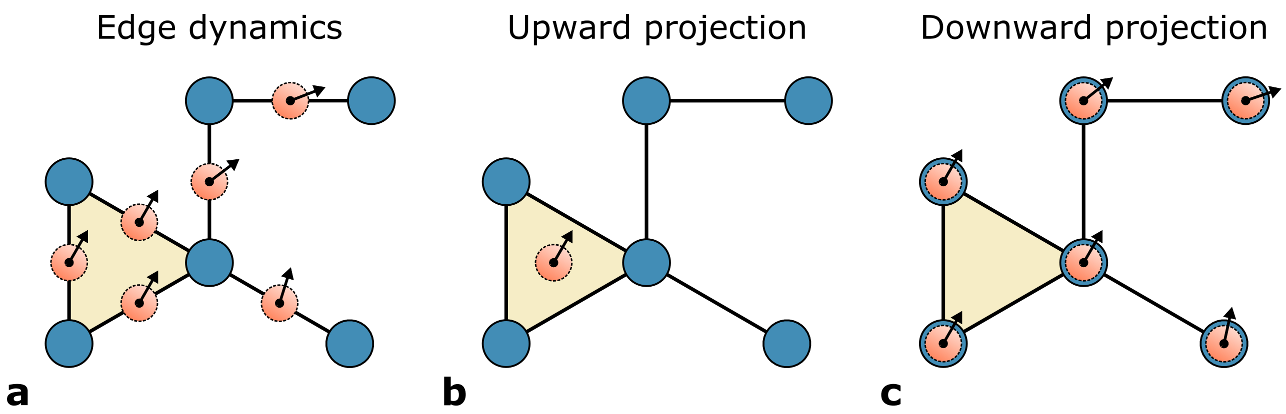
PERSPECTIVE
https://doi.org/10.1038/s41567-021-01371-4

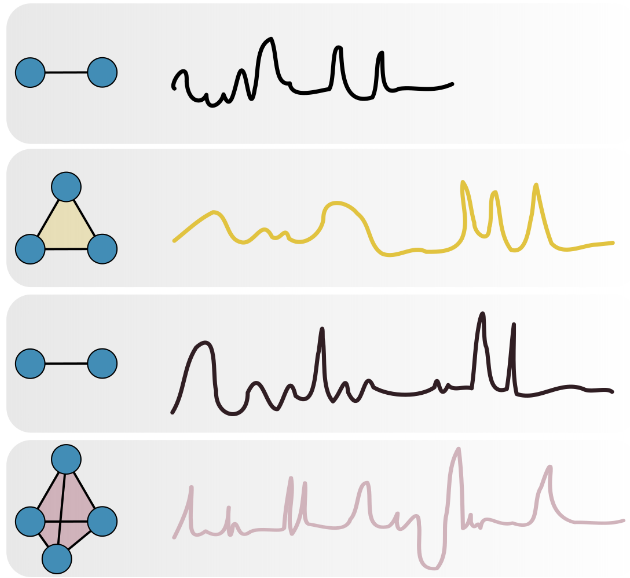
Check for updates

The physics of higher-order interactions in complex systems

Federico Battiston[1]✉, Enrico Amico[2,3], Alain Barrat[4,5], Ginestra Bianconi[6,7], Guilherme Ferraz de Arruda[8], Benedetta Franceschiello[9,10], Iacopo Iacopini[1], Sonia Kéfi[11,12], Vito Latora[6,13,14,15], Yamir Moreno[8,15,16,17], Micah M. Murray[9,10,18], Tiago P. Peixoto[1,19], Francesco Vaccarino[20] and Giovanni Petri[8,21]✉

Complex networks have become the main paradigm for modelling the dynamics of interacting systems. However, networks are intrinsically limited to describing pairwise interactions, whereas real-world systems are often characterized by higher-order interactions involving groups of three or more units. Higher-order structures, such as hypergraphs and simplicial complexes, are therefore a better tool to map the real organization of many social, biological and man-made systems. Here, we highlight recent evidence of collective behaviours induced by higher-order interactions, and we outline three key challenges for the physics of higher-order systems.





Outline of the course:
Introduction to Algebraic Topology

1. **Introduction to algebraic topology**
2. **Topological Kuramoto model**
3. **Dirac operator and Topological Dirac equation**
4. **Dirac and Global Topological synchronisation, Dirac Turing patterns**

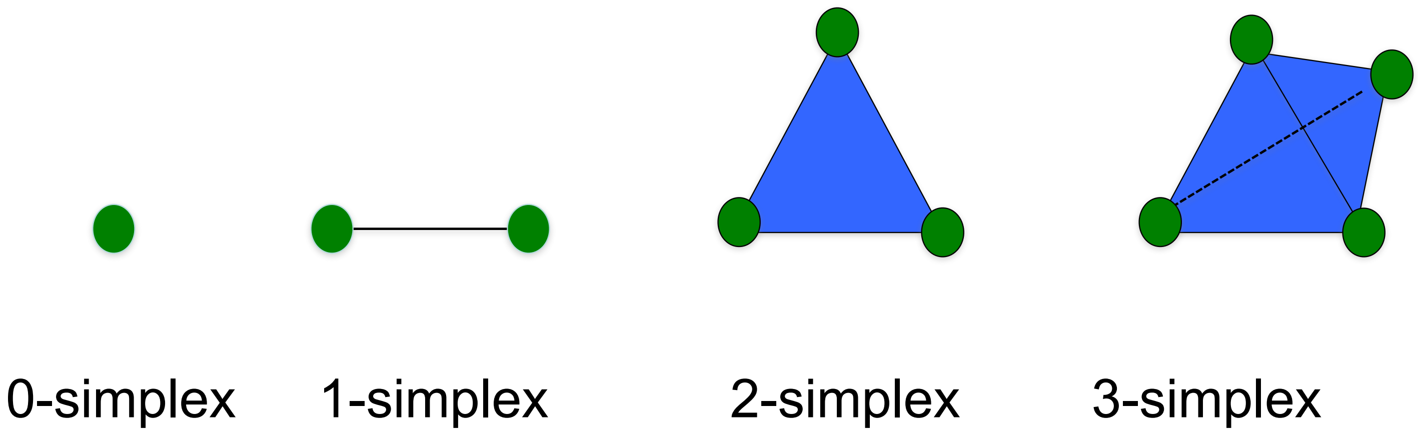
Lesson I:
Introduction to Algebraic Topology

- Introduction to simplicial complexes
- Introduction to algebraic topology
- Higher-order operators and their properties

1. Topological signals
2. Chains and Co-chains
3. The boundary and the co-boundary operator
4. The Hodge Laplacian and Hodge decomposition

Introduction to Simplicial complexes

Simplices



SIMPLICES

A d-dimensional simplex α (also indicated as a d-simplex α) is formed by a set of $(d+1)$ interacting nodes

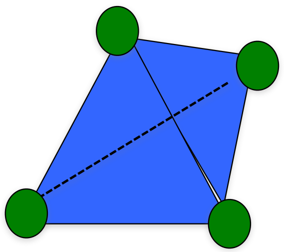
$$\alpha = [v_0, v_1, v_2 \ldots, v_d].$$

It describes a many body interaction between the nodes.
It allows for a topological and a geometrical interpretation of the simplex.

Faces of a simplex

FACES

A face of a d-dimensional simplex α is a simplex α' formed by a proper subset of nodes of the simplex, i.e. $\alpha' \subset \alpha$.

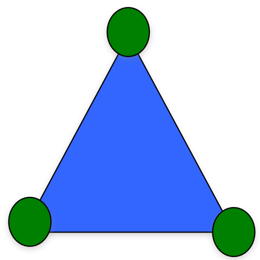


3-simplex

Faces

4 0-simplices

6 1-simplices

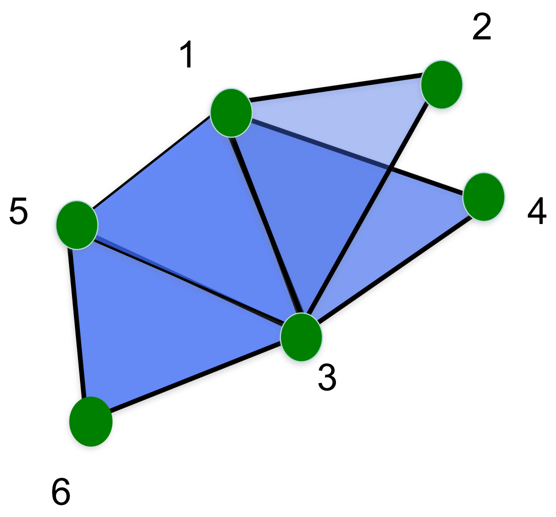


4 2-simplices

Simplicial complex

SIMPLICIAL COMPLEX

A simplicial complex $\mathcal{K}$ is formed by a set of simplices that is closed under the inclusion of the faces of each simplex.
The dimension d of a simplicial complex is the largest dimension of its simplices.

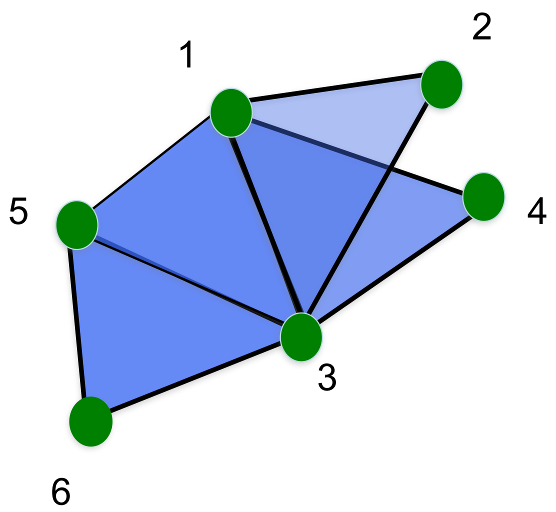


If a simplex α belongs to the simplicial complex $\mathscr{K}$ then every face of α must also belong to $\mathscr{K}$

$$\mathscr{K} = \{[1], [2], [3], [4], [5], [6], [1,2], [1,3], [1,4], [1,5], [2,3], [3,4], [3,5], [3,6], [5,6], [1,2,3], [1,3,4], [1,3,5], [3,5,6]\}$$

Dimension of a simplicial complex

The dimension of a simplicial complex $\mathscr{K}$
is the largest dimension of its simplices



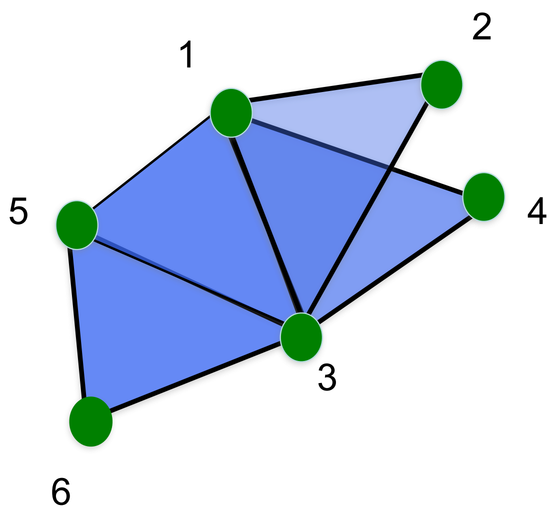
This simplicial complex has dimension 2

$$\mathscr{K} = \{[1], [2], [3], [4], [5], [6],\\ [1,2], [1,3], [1,4], [1,5], [2,3],\\ [3,4], [3,5], [3,6], [5,6],\\ [1,2,3], [1,3,4], [1,3,5], [3,5,6]\}$$

Facets of a simplicial complex

FACET

A facet is a simplex of a simplicial complex that is not a face of any other simplex. Therefore a simplicial complex is fully determined by the sequence of its facets.



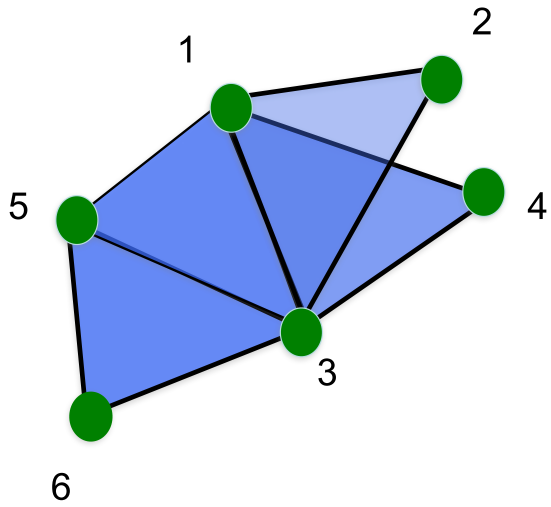
The facets of this simplicial complex are

$$\mathscr{K} = \{[1,2,3], [1,3,4], [1,3,5], [3,5,6]\}$$

Pure simplicial complex

PURE SIMPLICIAL COMPLEXES

A pure d-dimensional simplicial complex is formed by a set of d-dimensional simplices and their faces.
Therefore pure d-dimensional simplicial complexes admit as facets only d-dimensional simplices.

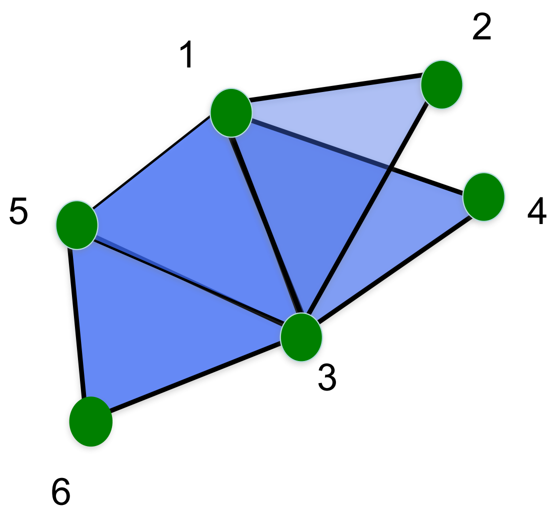


A pure d-dimensional simplicial complex is fully determined by an adjacency matrix tensor with (d+1) indices. For instance this simplicial complex is determined by the tensor

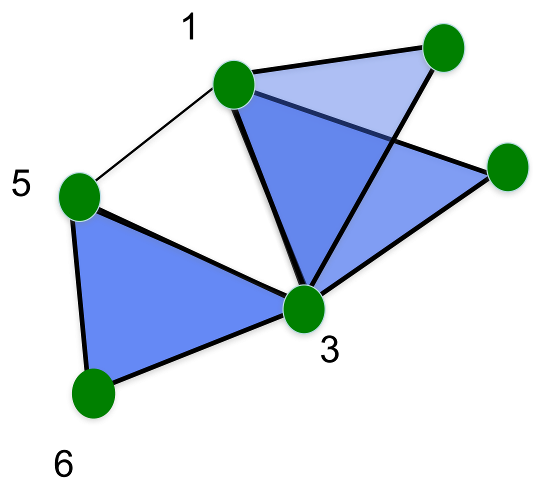
$$a_{rsp} = \begin{cases} 1 \text{ if } (r,s,p) \in \mathscr{K} \\ 0 \text{ otherwise} \end{cases}$$

Example

A simplicial complex $\mathscr{K}$ is pure
if it is formed by d-dimensional simplices
and their faces



PURE SIMPLICIAL COMPLEX



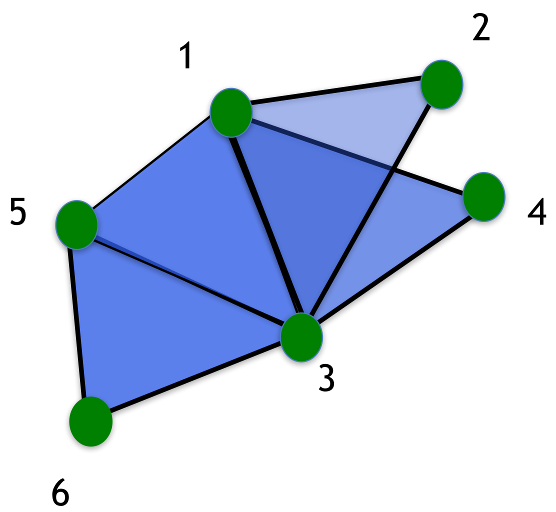
SIMPLICIAL COMPLEX THAT IS NOT PURE

Generalized degree

The generalized degree $k_{m',m}(\alpha)$of a m-face α

is given by the number

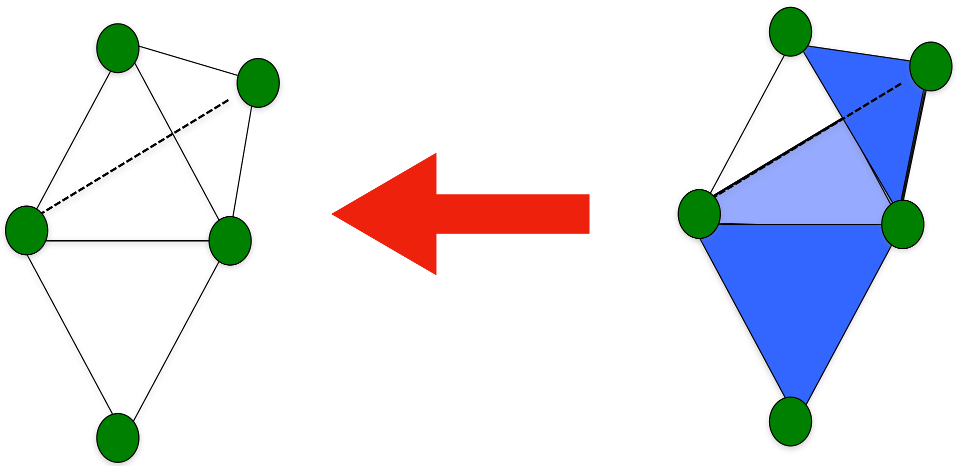
of m'-dimensional simplices incident to the m-face α.



r	$k_{2,0}([r])$
[1]	3
[2]	1
[3]	4
[4]	1
[5]	2
[6]	1

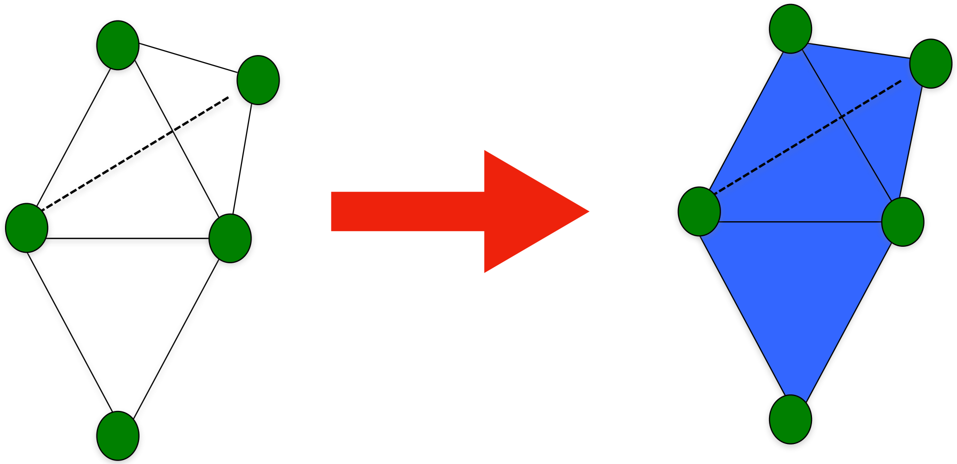
$[r,s]$	$k_{2,1}([r,s])$
[1,2]	1
[1,3]	3
[1,4]	1
[1,5]	1
[2,3]	1
[3,4]	1
[3,5]	2
[3,6]	1
[5,6]	1

Simplicial complex skeleton



From a simplicial complex is possible to generate a network salled the simplicial complex skeleton by considering only the nodes and the links of the simplicial complex

Clique complex



From a network is possible to generate a simplicial complex by Assuming that each clique is a simplex

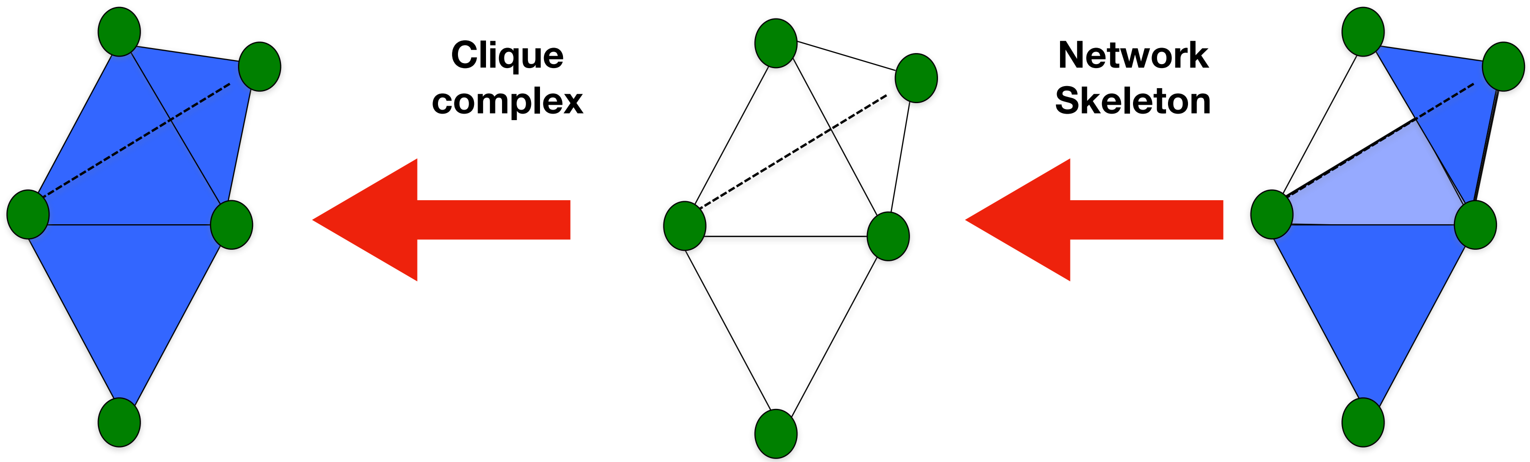
Note:

Poisson networks have a clique number that is 3 and actually on a finite expected number of triangles in the infinite network limit

However

Scale-free networks have a diverging clique number, therefore the clique complex of a scale-free network has diverging dimension. (Bianconi,Marsili 2006)

Concatenation of the operations



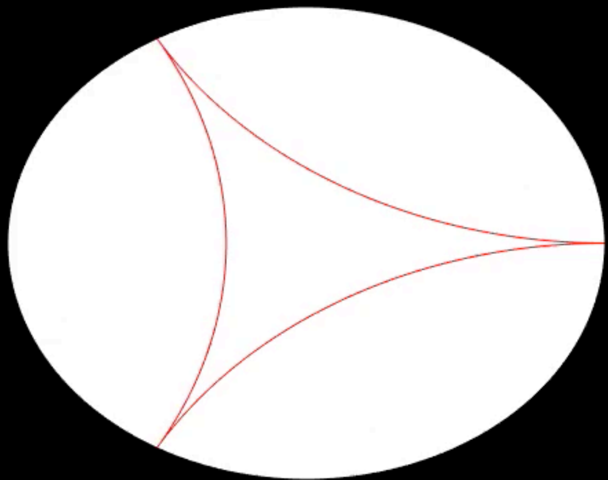
Attention!

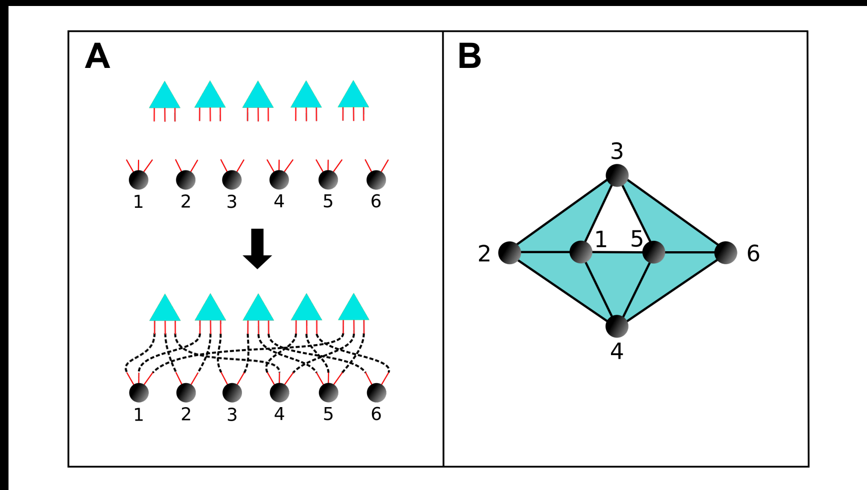
By concatenating the operations you are not guaranteed to return to the initial simplicial complex

Simplicial complex models

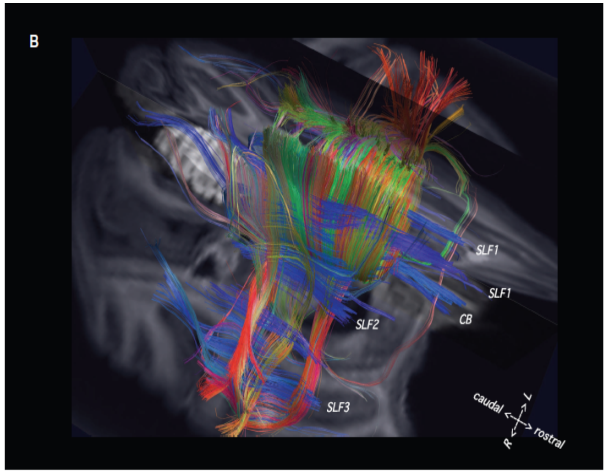
Emergent Geometry
Network Geometry with Flavor (NGF)
[Bianconi Rahmede ,2016 & 2017]

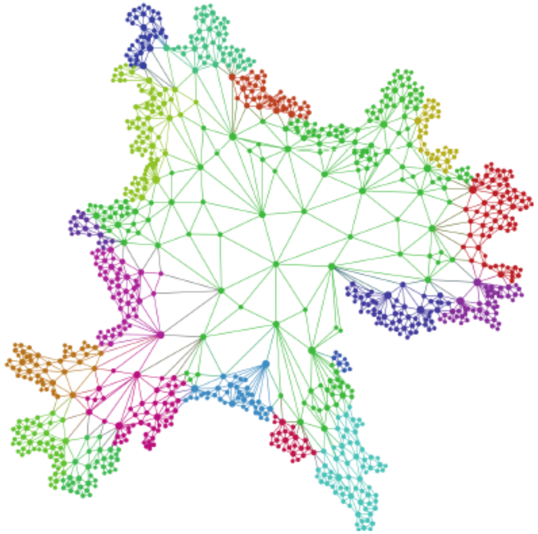
Maximum entropy model
Configuration model
of simplicial complexes
[Courtney Bianconi 2016]





Network Topology and Geometry



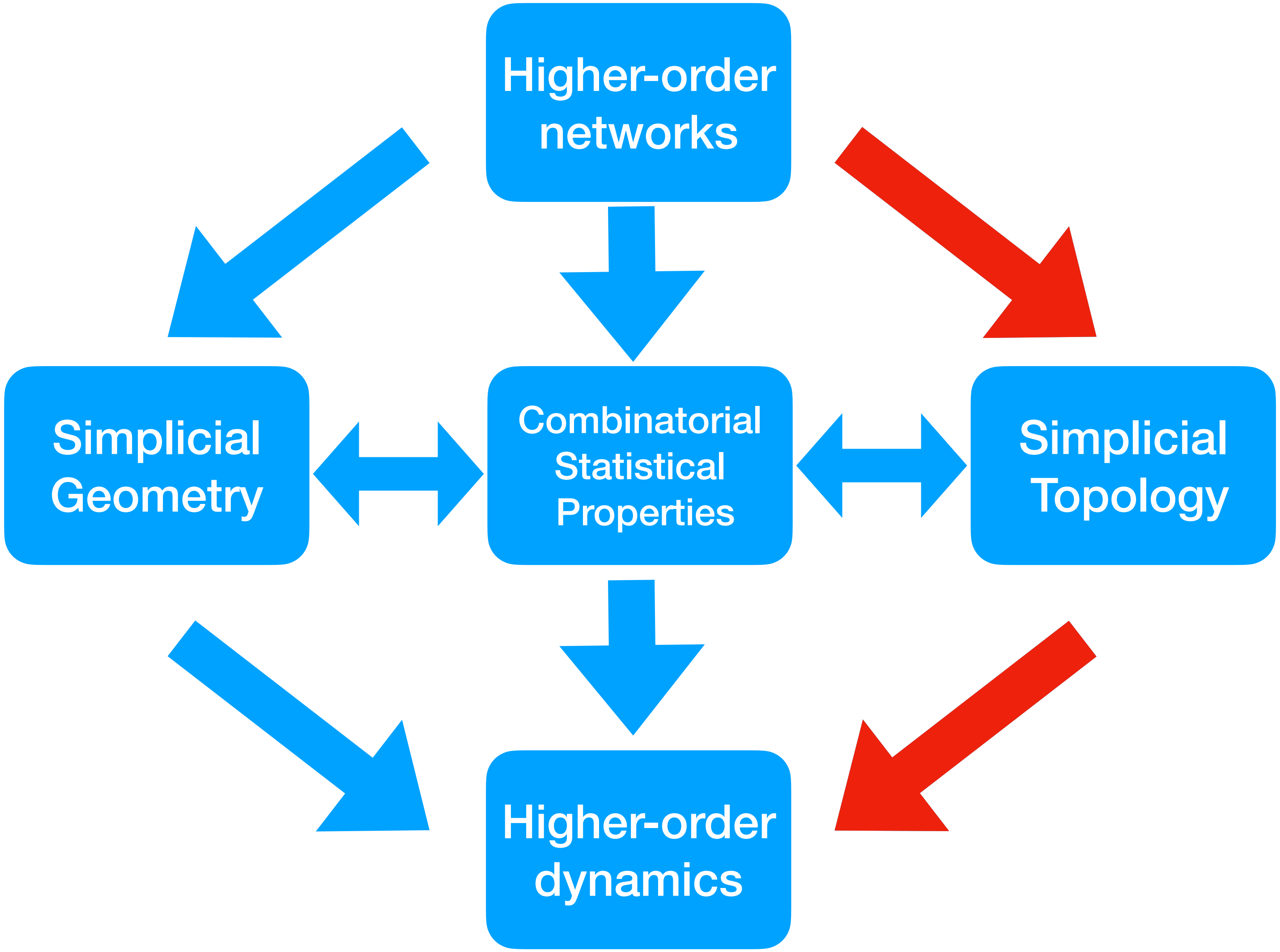


Are expected to have impact in a variety of applications,

ranging from

brain research to biological transportation networks

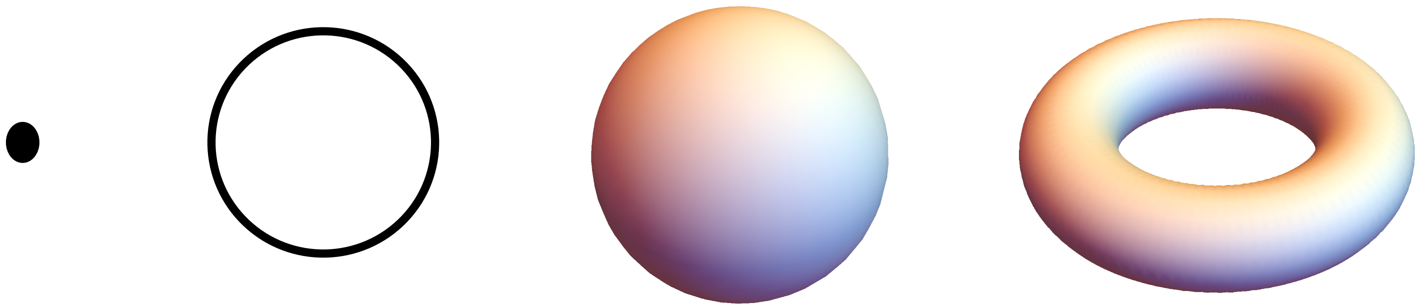
Higher-order structure and dynamics



Introduction to Algebraic Topology

Betti numbers

Point **Circle** **Sphere** **Torus**

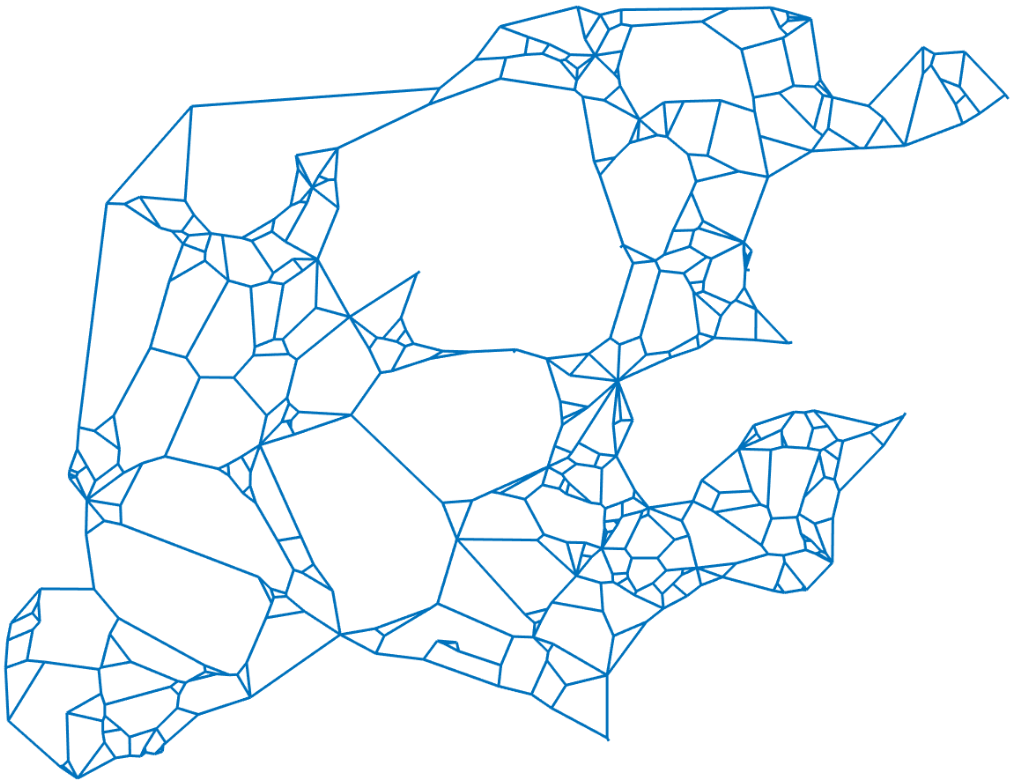


Point	Circle	Sphere	Torus
$\beta_0 = 1$	$\beta_0 = 1$	$\beta_0 = 1$	$\beta_0 = 1$
$\beta_1 = 0$	$\beta_1 = 1$	$\beta_1 = 0$	$\beta_1 = 2$
$\beta_2 = 0$	$\beta_2 = 0$	$\beta_2 = 1$	$\beta_2 = 1$

Euler characteristic

$$\chi = \sum_{m=0}^{d} (-1)^m \beta_m$$

Betti number 1



Fungi network from Sang Hoon Lee, et. al. Jour. Compl. Net. (2016)

Simplicial complex:notation

We consider a d-dimensional simplicial complex $\mathscr{K}$ having N_m

positively oriented simplices α_r^m

(or simply r) of dimension m.

We indicate the set of all the m positively oriented simplices of the simplicial complex $Q_m(\mathscr{K})$

Orientation of a simplex

A m-dimensional *oriented simplex* α is a set of $m+1$ nodes

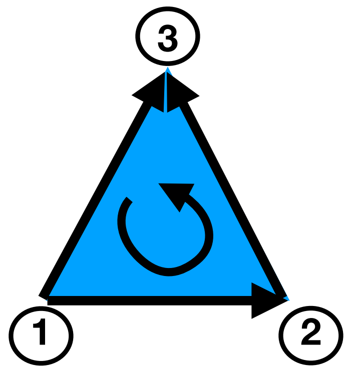
$$\alpha = [v_0, v_1, \ldots, v_m], \tag{3.1}$$

associated to an orientation wuch that

$$[v_0, v_1, \ldots, v_m] = (-1)^{\sigma(\pi)}[v_{\pi(0)}, v_{\pi(1)}, \ldots, v_{\pi(m)}] \tag{3.2}$$

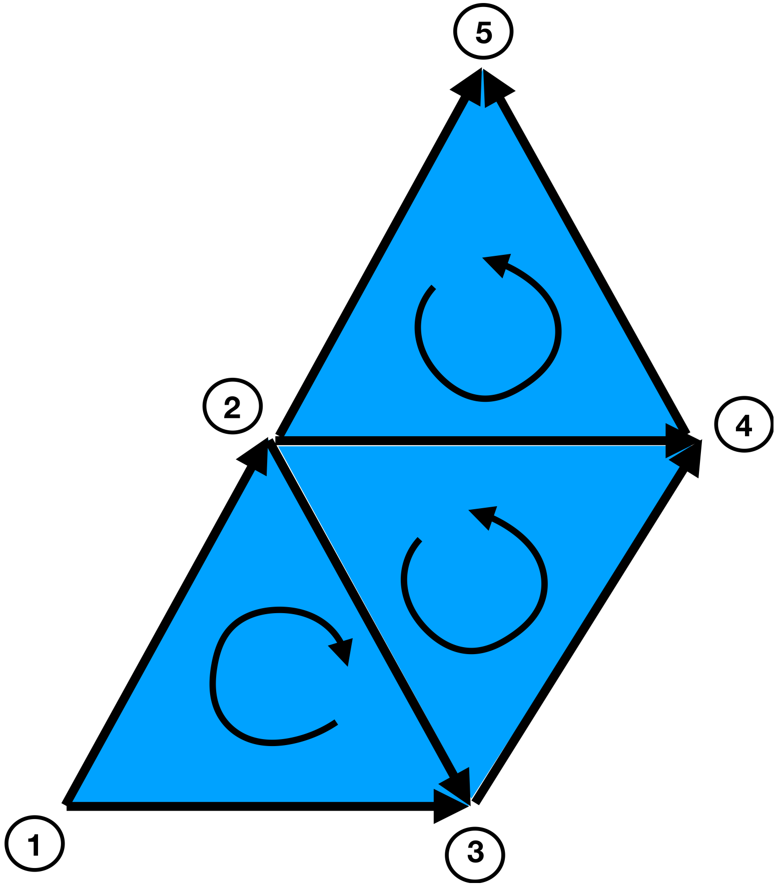
where $\sigma(\pi)$ indicates the parity of the permutation π.

$[r, s] = -[s, r]$



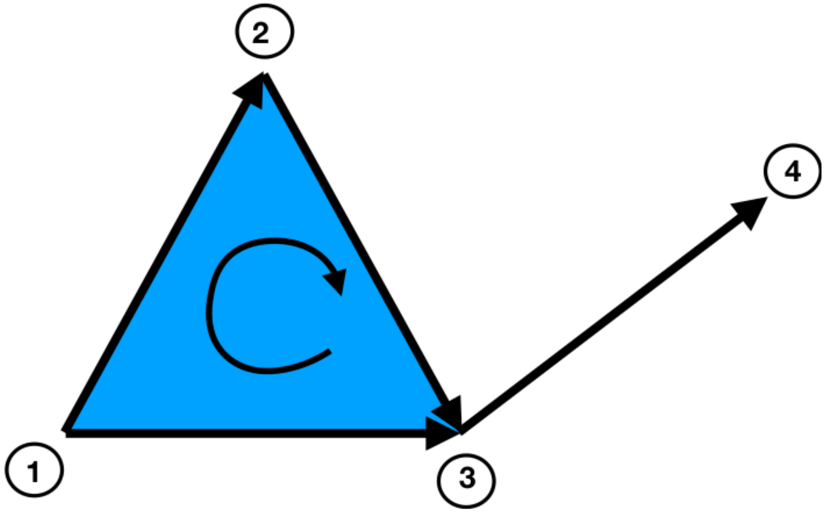
$[r, s, q] = [s, q, r] = [q, r, s] = -[s, r, q] = -[q, s, r] = -[r, q, s]$

Oriented simplicial complex



A typical choice of orientation of a simplicial complex, is to consider the orientation induced by the node labels, i.e. each simplex is oriented in an increasing (or decreasing) order of the node labels

Oriented simplicial complex



The set of positively oriented simplices on this simplicial complex are:

{[1,2,3], [1,2], [2,3], [1,3], [3,4], [1], [2], [3], [4]}

We adopt the convention that each 0-simplex is positively oriented

m-Chains

THE m-CHAINS

Given a simplicial complex, a m-chain C_m consists of the elements of a free abelian group with basis on the m-simplices of the simplicial complex.

Its elements can be represented as linear combinations of the of all oriented m-simplices

$$\alpha = [v_0, v_1, \ldots, v_m] \tag{3.6}$$

with coefficients in $\mathbb{Z}$.

m-chain $c_m \in C_m$

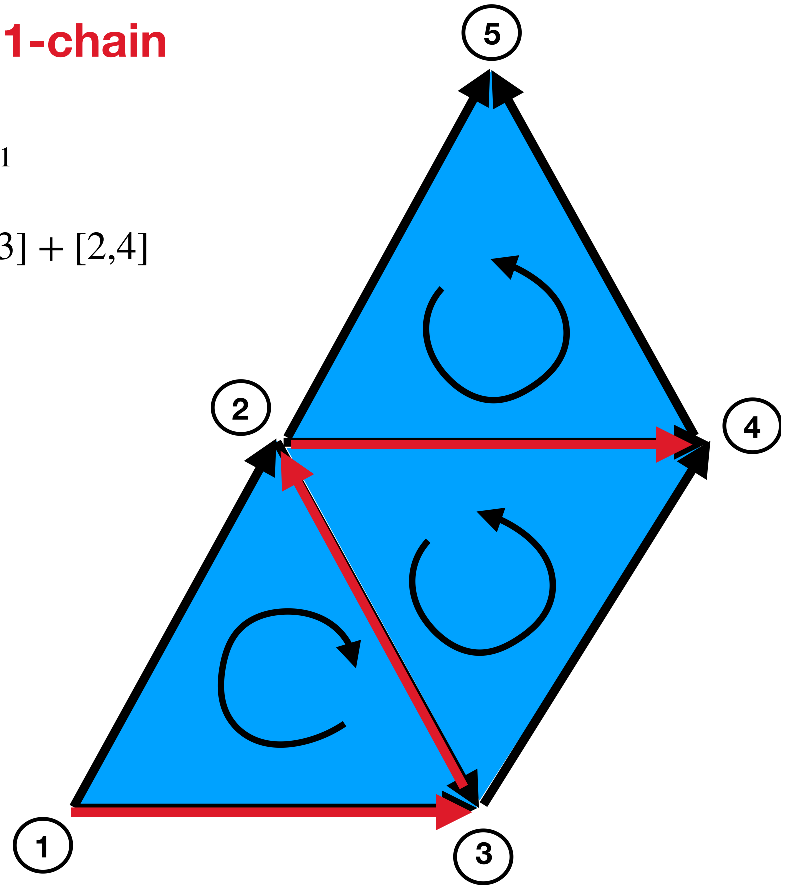
$$c_m = \sum_{\alpha_r \in Q_m(\mathcal{K})} c_m^r \alpha_r^m, \text{ **with** } c_m^r \in \mathbb{Z}$$

Oriented simplicial complex and m-chains

Example of 1-chain

$a \in \mathscr{C}_1$

$a = [1,3] - [2,3] + [2,4]$



Boundary operator

THE BOUNDARY MAP

The boundary map ∂_m is a linear operator

$$\partial_m : C_m \to C_{m-1} \tag{3.8}$$

whose action is determined by the action on each m-simplex of the simplicial complex is given by

$$\partial_m[v_0, v_1 \ldots, v_m] = \sum_{p=0}^{m} (-1)^p [v_0, v_1, \ldots, v_{p-1}, v_{p+1}, \ldots, v_m]. \tag{3.9}$$

Boundary operator

The boundary map ∂_n is a linear operator

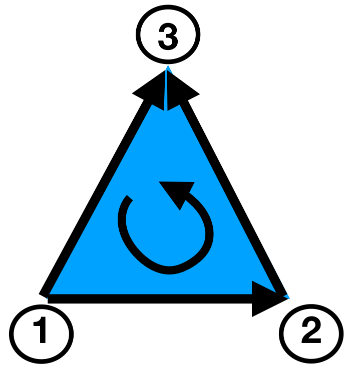
$$\partial_m : \mathscr{C}_m \to \mathscr{C}_{m-1}$$

whose action is determined by the action on each n-simplex of the simplicial complex

$$\partial_m[v_0, v_1 \ldots, v_m] = \sum_{p=0}^{m} (-1)^p [v_0, v_1, \ldots, v_{p-1}, v_{p+1}, \ldots, v_m] \, .$$

Therefore we have

$$\partial_1[1,2] = [2] - [1] \, .$$



$$\partial_2[1,2,3] = [2,3] - [1,3] + [1,2] \, .$$

Boundary operator

THE BOUNDARY MAP

The boundary map ∂_m is a linear operator

$$\partial_m : C_m \to C_{m-1} \tag{3.8}$$

whose action is determined by the action on each m-simplex of the simplicial complex is given by

$$\partial_m[v_0, v_1 \ldots, v_m] = \sum_{p=0}^{m} (-1)^p [v_0, v_1, \ldots, v_{p-1}, v_{p+1}, \ldots, v_m]. \tag{3.9}$$

From this definition it follows that the $\mathrm{im}(\partial_m)$ corresponds to the space of $(m-1)$ boundaries and the $\ker(\partial_m)$ is formed by the cyclic m-chains.

Special groups

Boundary group $\hat{B}_m = \mathbf{im}(\partial_{m+1})$
Cycle group $\hat{Z}_m = \mathbf{ker}(\partial_m)$

The boundary of a boundary is null

The boundary operator has the property

$$\partial_m \partial_{m+1} = 0 \quad \forall m \geq 1$$

Which is usually indicated by saying that the boundary of the boundary is null.

This property follows directly from the definition of the boundary, as an example we have

$$\partial_1 \partial_2 [r, s, q] = \partial_1([r, s] + [s, q] - [r, q]) = [s] - [r] + [q] - [s] - [q] + [r] = 0.$$

Proof

The boundary of the boundary is null.

Proof: Indicating with $\hat{v}_p$ the p[th] missing vertex we have

$$\partial_{m-1}\partial_m[v_0, v_1, \ldots, v_m] = \sum_{p=0}^{m} (-1)^p \partial_{m-1}[v_0, v_1, \ldots \hat{v}_p \ldots v_m]$$

$$= \sum_{p=0}^{m} (-1)^p \sum_{p'=0}^{p-1} (-1)^{p'} [v_0, v_1, \ldots \hat{v}_{p'} \ldots \hat{v}_p \ldots v_m]$$

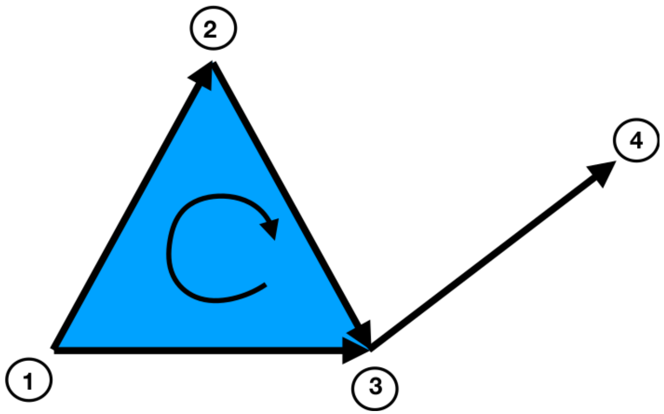
$$+ \sum_{p=0}^{m} (-1)^p \sum_{p'=p+1}^{m} (-1)^{p'-1} [v_0, v_1, \ldots \hat{v}_p \ldots \hat{v}_{p'} \ldots v_m] = 0$$

Incidence matrices

Given a basis for the m simplices and m-1 simplices
the m-boundary operator

$$\partial_m[v_0, v_1 \ldots, v_m] = \sum_{p=0}^{m} (-1)^p [v_0, v_1, \ldots, v_{p-1}, v_{p+1}, \ldots, v_m] \,.$$

is captured by the $N_{m-1} \times N_m$ **incidence (or boundary) matrix** $\mathbf{B}_{[m]}$



$$\mathbf{B}_{[1]} = \begin{array}{c|cccc} & [1,2] & [1,3] & [2,3] & [3,4] \\ [1] & -1 & -1 & 0 & 0 \\ [2] & 1 & 0 & -1 & 0 \\ [3] & 0 & 1 & 1 & -1 \\ [4] & 0 & 0 & 0 & 1 \end{array} \,,$$

$$\mathbf{B}_{[2]} = \begin{array}{c|c} & [1,2,3] \\ [1,2] & 1 \\ [1,3] & -1 \\ [2,3] & 1 \\ [3,4] & 0 \end{array} \,.$$

Boundary of the boundary is null

In terms of the incidence matrices the relation

$$\partial_m \partial_{m+1} = 0 \quad \forall m \geq 1$$

Can be expressed as

$$\mathbf{B}_{[m]}\mathbf{B}_{[m+1]} = \mathbf{0} \quad \forall m \geq 1 \qquad \mathbf{B}_{[m+1]}^{\top}\mathbf{B}_{[m]}^{\top} = \mathbf{0} \quad \forall m \geq 1$$

Homology groups

THE HOMOLOGY GROUPS

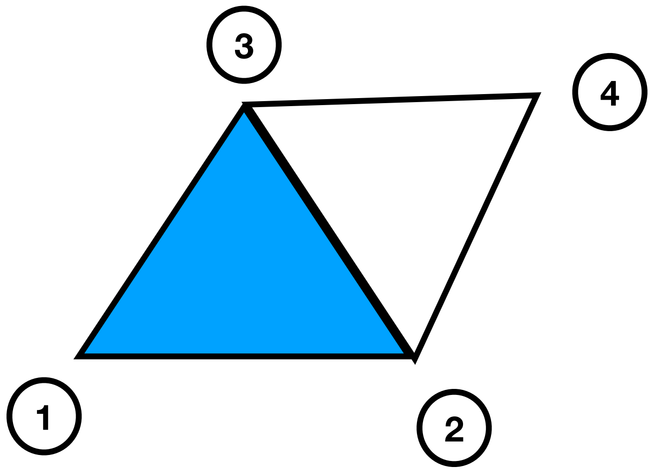
The homology group $\mathcal{H}_m$ is the quotient space

$$\mathcal{H}_m = \frac{\ker(\partial_m)}{\mathrm{im}(\partial_{m+1})}, \tag{3.14}$$

denoting homology classes of m-cyclic chains that are in the $\ker(\partial_m)$ and they do differ by cyclic chains that are not boundaries of $(m+1)$-chains, i.e. they are in $\mathrm{im}(\partial_{m+1})$.

It follows that $a \in$ ker(∂_m) is in the same homology class than $a + b \in$ ker(∂_m) with $b \in$ im(∂_{m+1})

Homology



$$\mathscr{H}_1 = \mathbb{Z}$$

The two 1-chains

$$a = [2,4] - [3,4] - [2,3]$$

$$b = [1,2] + [2,4] - [3,4] - [1,3]$$

are in the same homology class

$$a \sim b$$

in fact

$$b = a + \partial_2[1,2,3] = [2,4] - [3,4] - [2,3] + [1,2] + [2,3] - [1,3]$$

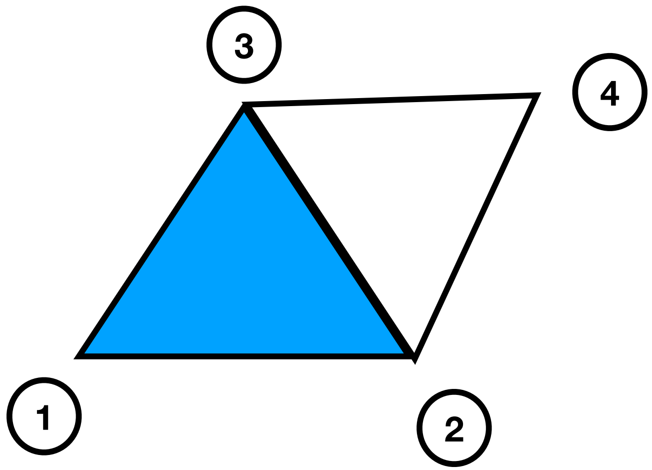
Betti numbers

BETTI NUMBERS

The Betti number β_m indicates the number of m-dimensional cavities of a simplicial complex and is given by the rank of the homology group $\mathcal{H}_m$, i.e.

$$\beta_m = \text{rank}(\mathcal{H}_m) = \text{rank}(\ker(\partial_m)) - \text{rank}(\text{im}(\partial_{m+1})). \tag{3.15}$$

Betti number



$$\mathscr{H}_1 = \mathbb{Z}$$

$$\beta_1 = \mathbf{dim}\mathscr{H}_1 = 1$$

The two 1-chains

$$a = [2{,}4] - [3{,}4] - [2{,}3]$$

$$b = [1{,}2] + [2{,}4] - [3{,}4] - [1{,}3]$$

are in the same homology class

$$a \sim b$$

in fact

$$b = a + \partial_2[1{,}2{,}3] = [2{,}4] - [3{,}4] - [2{,}3] + [1{,}2] + [2{,}3] - [1{,}3]$$

Euler characteristic

THE EULER CHARACTERISTIC AND THE EULER-POINCARÉ FORMULA

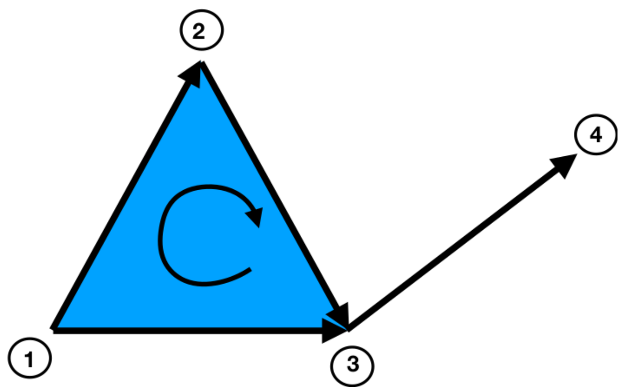
The Euler characterisic χ is defined as the alternating sum of the number of m-dimensional simplices, i.e.

$$\chi = \sum_{m \geq 0} s_m, \tag{3.16}$$

where s_m is the number of m-dimensional simplices in the simplicial complex. According to the Euler-Poincaré formula, the Euler characteristic χ of a simplicial complex can be expressed in terms of the Betti numbers as

$$\chi = \sum_{m \geq 0} (-1)^m \beta_m. \tag{3.17}$$

Boundary Operators



Boundary operators

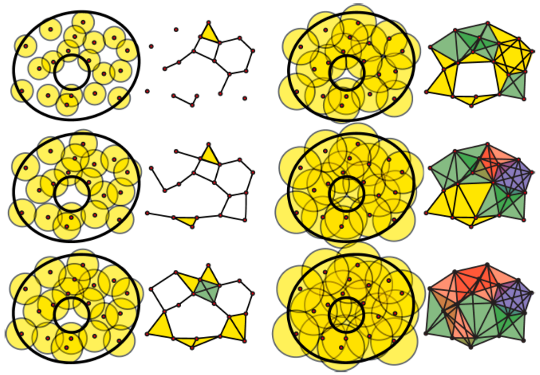
$$\mathbf{B}_{[1]} = \begin{array}{c|cccc} & [1,2] & [1,3] & [2,3] & [3,4] \\ [1] & -1 & -1 & 0 & 0 \\ [2] & 1 & 0 & -1 & 0 \\ [3] & 0 & 1 & 1 & -1 \\ [4] & 0 & 0 & 0 & 1 \end{array}, \qquad \mathbf{B}_{[2]} = \begin{array}{c|c} & [1,2,3] \\ [1,2] & 1 \\ [1,3] & -1 \\ [2,3] & 1 \\ [3,4] & 0 \end{array}.$$

The boundary of the boundary is null

$$\mathbf{B}_{[m-1]}\mathbf{B}_{[m]} = \mathbf{0}, \quad \mathbf{B}_{[m]}^\top \mathbf{B}_{[m-1]}^\top = \mathbf{0}$$

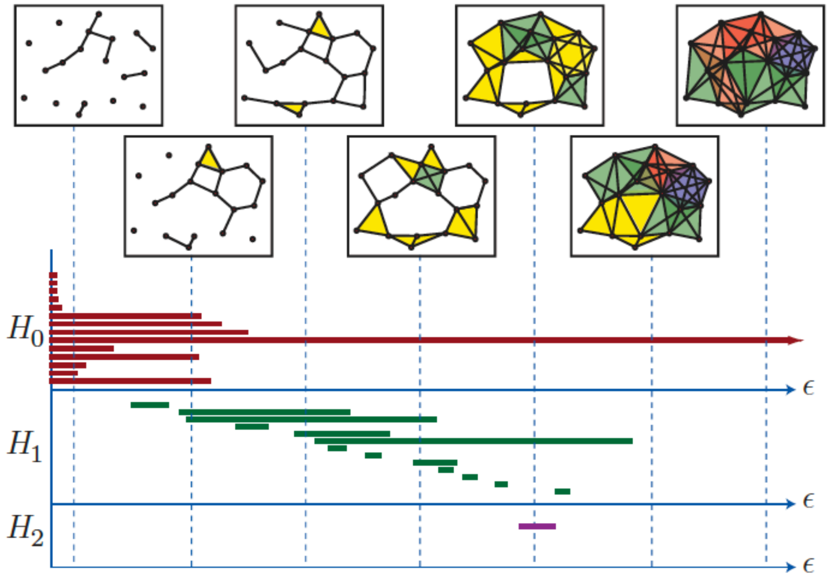
Persistent homology

Filtration: distance/weights



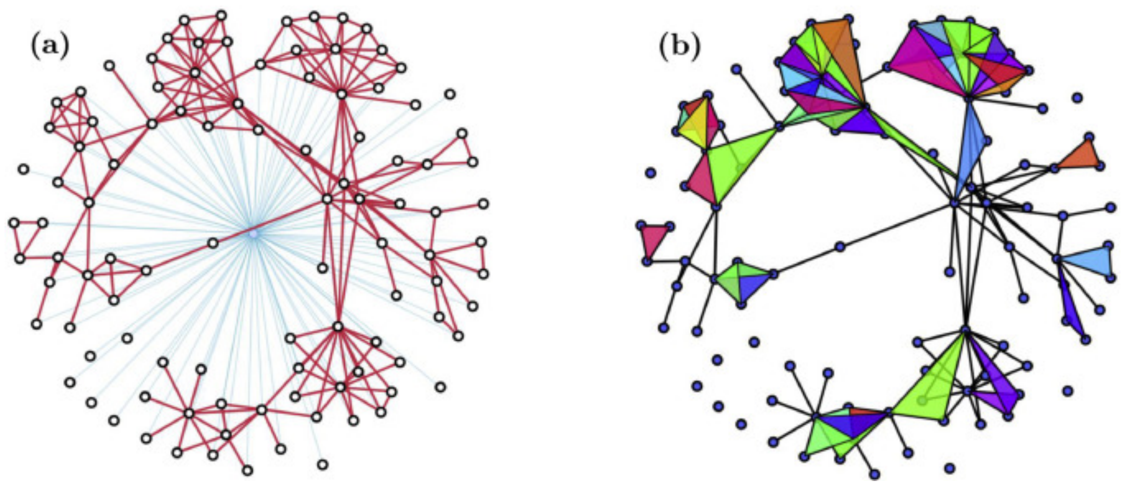
Ghrist 2008

Persistent homology Barcode



Topological clustering

The node neighbourhood is the clique simplicial complex formed by the set of all the neighbours of a node and their connections



Properties of the node

The degree k_r

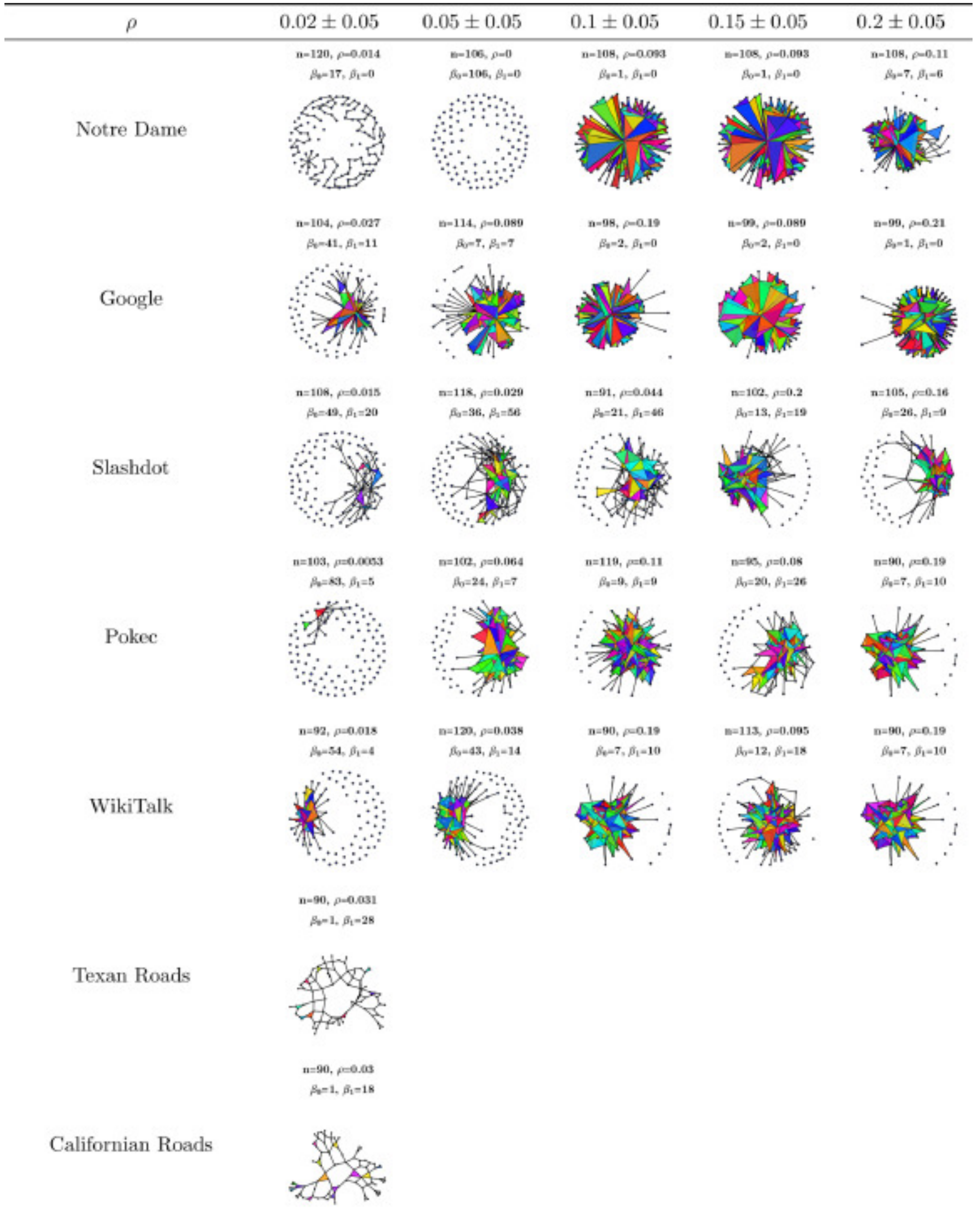
The local clustering coefficient C_r

AP Kartun-Giles et al. (2019)

Properties of the node neighbourhood

Number of nodes n

Density of the links ρ



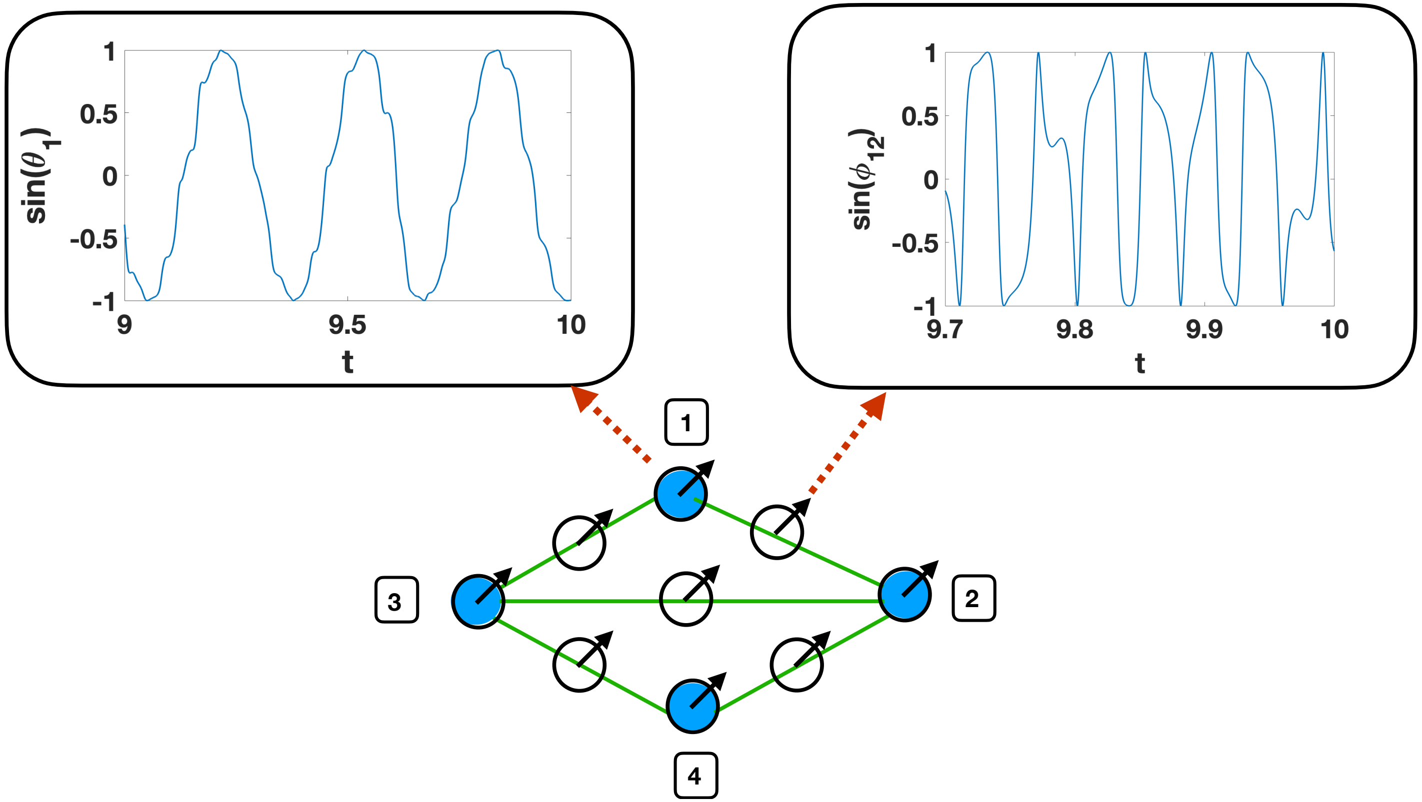
Node neighbourhoods with the same number of nodes and the same density of links can have very different topology

AP Kartun-Giles et al. (2019)

Topological signals,
coboundary operators

Topological signals

Simplicial complexes and networks can sustain dynamical variables (signals) not only defined on nodes but also defined on higher order simplices these signals are called *topological signals*

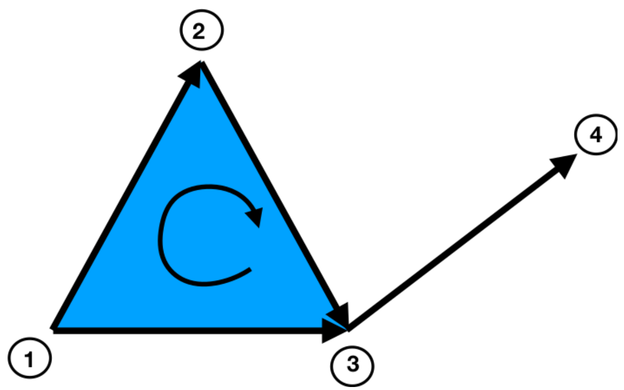


Topological signals

- Citations in a collaboration network
- Speed of wind at given locations
- Currents at given locations in the ocean
- Fluxes in biological transportation networks
- Synaptic signal
- Edge signals in the brain

Topological signals
are cochains or vector fields

Boundary Operators



Boundary operators

$$\mathbf{B}_{[1]} = \begin{array}{c|cccc} & [1,2] & [1,3] & [2,3] & [3,4] \\ \hline [1] & -1 & -1 & 0 & 0 \\ [2] & 1 & 0 & -1 & 0 \\ [3] & 0 & 1 & 1 & -1 \\ [4] & 0 & 0 & 0 & 1 \end{array}, \qquad \mathbf{B}_{[2]} = \begin{array}{c|c} & [1,2,3] \\ \hline [1,2] & 1 \\ [1,3] & -1 \\ [2,3] & 1 \\ [3,4] & 0 \end{array}.$$

$\mathbf{B}_{[1]}$ **Discrete divergence**

$\mathbf{B}_{[1]}^{\top}$ **Discrete gradient**

$\mathbf{B}_{[2]}^{\top}$ **Discrete Curl**

The boundary of the boundary is null

$$\mathbf{B}_{[m-1]}\mathbf{B}_{[m]} = \mathbf{0}, \quad \mathbf{B}_{[m]}^{\top}\mathbf{B}_{[m-1]}^{\top} = \mathbf{0}$$

Cochains

m-cochains

A m-dimensional cochain $f \in C^m$ is a linear function $f : C_m \rightarrow \mathbb{R}$, that associates to every m-chain of the simplicial complex a value in $\mathbb{R}$.

m-cochain $f \in C^m$

Given the m-chain $c_m \in C_m$

$$c_m = \sum_{r \in Q_m(\mathcal{K})} c_m^r \alpha_r^m, \text{ with } c_m^r \in \mathbb{Z}$$

$$f(c_m) = \sum_{r \in Q_m(\mathcal{K})} c_m^r f([\alpha_r^m]), \text{ with } c_m^r \in \mathbb{Z}$$

Oriented simplicial complex and m-chains

Example of 1-chain

$$a \in \mathscr{C}_1$$

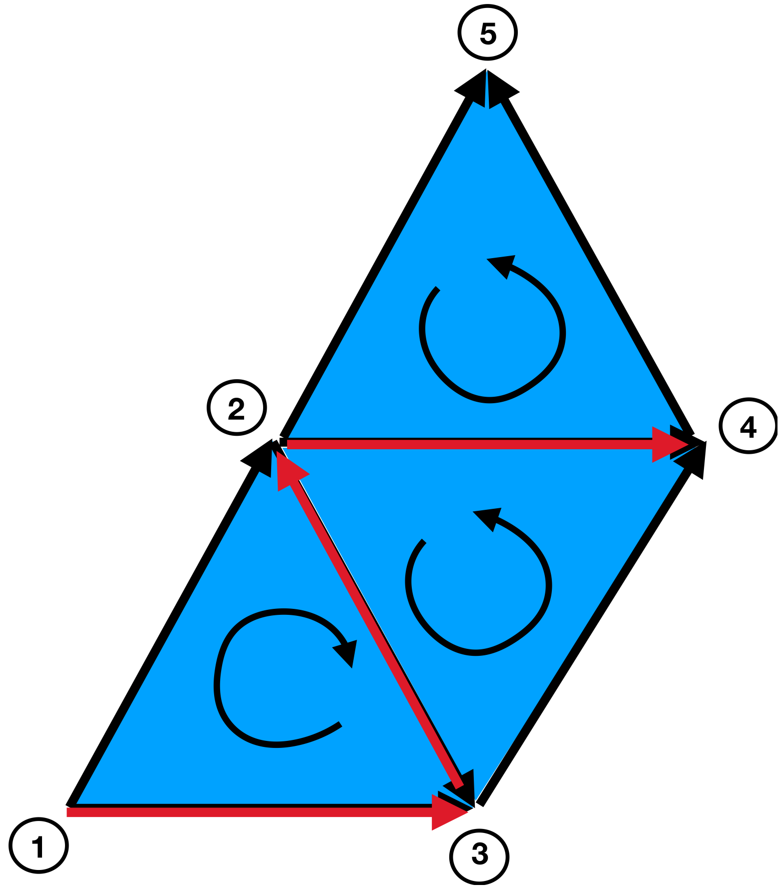
$$a = [1,3] - [2,3] + [2,4]$$

Example

Given $f \in C^1$

then

$$f(a) = f([1,3]) - f([2,3]) + f([2,4])$$



Cochains:properties

m-cochains

A m-dimensional cochain $f \in C^m$ is a linear function $f : C_m \to \mathbb{R}$, that associates to every m-chain of the simplicial complex a value in $\mathbb{R}$.

Upon a change of orientation of a simplex the value of the cochain associated to a simplex changes sign

$$f([\alpha_r^m]) = -f(-[\alpha_r^m]) \ \forall \alpha_r^m \in \mathcal{Q}_m(\mathcal{K})$$

For $m = 1$ a cochain can for instance express a flux along the links of the simplicial complex

Cochains:properties

m-cochains

A m-dimensional cochain $f \in C^m$ is a linear function $f : C_m \longrightarrow \mathbb{R}$, that associates to every m-chain of the simplicial complex a value in $\mathbb{R}$.

Given a basis for the m-simplices of the simplicial complex,
A m-cochain can be expressed as a vector $\mathbf{f}$ of elements

$$f_r = f([\alpha_r^m]) \ \forall \alpha_r^m \in Q_m(\mathscr{K})$$

L^2 norm between cochains

We define a scalar product between m-cochains as

$$\langle f, f \rangle = \mathbf{f}^\top \mathbf{f}$$

Which has an element by element expression

$$\langle f, f \rangle = \sum_{r \in Q_m(\mathscr{K})} f_r^2$$

This scalar product can be generalised by introducing metric matrices (see lecture III)

Coboundary operator

Coboundary operator δ_m

The coboundary operator $\delta_m : C^m \rightarrow C^{m+1}$ associates to every m-cochain of the simplicial complex $(m+1)$-cochain

$$\delta_m f = f \circ \partial_{m+1}.$$

Therefore we obtain

$$(\delta_m f)[v_0, v_1, \ldots, v_{m+1}] = \sum_{p=0}^{m+1} (-1)^p f([v_0, v_1, \ldots, v_{p-1}, v_{p+1} \ldots v_{m+1}])$$

If follows that if $g \in C^{m+1}$ is given by $g = \delta_m f$.

Then $\mathbf{g} = \mathbf{B}_{m+1}^{\top}\mathbf{f} \equiv \bar{\mathbf{B}}_{m+1}\mathbf{f}$

Coboundary operator

Coboundary operator δ_m

The coboundary operator $\delta_m : C^m \to C^{m+1}$ associates to every m-cochain of the simplicial complex $(m+1)$-cochain

$$\delta_m f = f \circ \partial_{m+1}.$$

Therefore we obtain

$$(\delta_m f)[v_0, v_1, \ldots, v_{m+1}] = \sum_{p=0}^{m+1} (-1)^p f([v_0, v_1, \ldots, v_{p-1}, v_{p+1} \ldots v_{m+1}])$$

if follows that

$\delta_{m+1} \circ \delta_m = 0 \ \forall m \geq 1$ hence $\mathbf{B}^\top_{[m+1]} \mathbf{B}^\top_{[m]} = \mathbf{0}$

Discrete Gradient

If $f \in C^0$, then $g = \delta_1 f \in C^1$ indicates its discrete gradient

Indeed we have

$$\mathbf{g} = \mathbf{B}_{[1]}^{\top}\mathbf{f}$$

which implies

$$g_{[r,s]} = f_s - f_r$$

Discrete Curl

If $f \in C^1$, then $g = \delta_2 f \in C^2$ indicates its discrete curl

Indeed we have

$$\mathbf{g} = \mathbf{B}_{[2]}^{\top}\mathbf{f}$$

which implies

$$g_{[r,s,q]} = f_{[r,s]} + f_{[s,q]} - f_{[r,q]}$$

Adjoint of the coboundary operator

Adjoint operator δ_m^*

The adjont of the coboundary operator $\delta_m^* : C^{m+1} \to C^m$ satisfies

$$\langle g, \delta_m f \rangle = \left\langle \delta_m^* g, f \right\rangle$$

for any $f \in C^m$ and $g \in C^{m+1}$.

It follows that if $f' = \delta_m^* g$ then $\mathbf{f}' = \mathbf{B}_{[m+1]}\mathbf{g}$

Adjoint of the coboundary operator

Adjoint operator δ_m^*

The adjont of the coboundary operator $\delta_m^* : C^{m+1} \to C^m$ satisfies

$$\langle g, \delta_m f \rangle = \left\langle \delta_m^* g, f \right\rangle$$

where $f \in C^m$ and $g \in C^{m+1}$.

If follows that if $f' \in C^m$ is given by $f' = \delta_m^* g$.

Then $\mathbf{f}' = \bar{\mathbf{B}}_{[m+1]}^\top \mathbf{g} = \mathbf{B}_{[m+1]} \mathbf{g}$

Discrete Divergence

If $g \in C^1$, then $f = \delta_0^* g \in C^0$ indicates its discrete divergence

Indeed we have

$$\mathbf{f} = \mathbf{B}_{[1]}\mathbf{g}$$

which implies

$$f_r = \sum_s g_{[sr]} - \sum_s g_{[rs]}$$

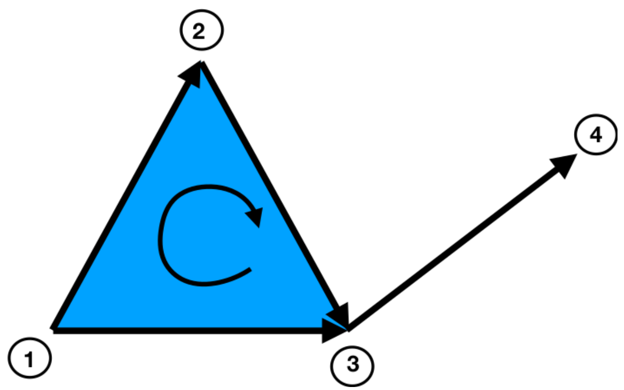
Coboundary action

In summary, the coboundary operator and its adjoint act on the cochains according to the following diagram

$$C^{m+1} \xleftarrow{\delta_m} C^m \xleftarrow{\delta_{m-1}} C^{m-1}$$

$$C^{m+1} \xrightarrow{\delta_m^*} C^m \xrightarrow{\delta_{m-1}^*} C^{m-1}$$

Boundary Operators



Boundary operators

$\mathbf{B}_{[1]} =$

	[1,2]	[1,3]	[2,3]	[3,4]
[1]	−1	−1	0	0
[2]	1	0	−1	0
[3]	0	1	1	−1
[4]	0	0	0	1

,

$\mathbf{B}_{[2]} =$

	[1,2,3]
[1,2]	1
[1,3]	−1
[2,3]	1
[3,4]	0

.

$\mathbf{B}_{[1]}$ Discrete divergence

$\mathbf{B}_{[1]}^{\top}$ Discrete gradient

$\mathbf{B}_{[2]}^{\top}$ Discrete Curl

The boundary of the boundary is null

$$\mathbf{B}_{[m-1]}\mathbf{B}_{[m]} = \mathbf{0}, \quad \mathbf{B}_{[m]}^{\top}\mathbf{B}_{[m-1]}^{\top} = \mathbf{0}$$

Hodge Laplacians

Hodge Laplacian

The Hodge-Laplacians

The m-dimensional Hodge-Laplacian L_m is defined as

$$L_m = L_m^{up} + L_m^{down}$$

where up and down m-dimensional Hodge Laplacians are given by

$$\begin{aligned} L_m^{up} &= \delta_m^* \delta_m, \\ L_m^{down} &= \delta_{m-1} \delta_{m-1}^*. \end{aligned}$$

Graph Laplacian in terms of the boundary matrix

The graph Laplacian of elements

$$\left(L_{[0]}\right)_{rs} = \delta_{rs} k_r - a_{rs}$$

Can be expressed in terms of the 1-incidence matrix

as

$$\mathbf{L}_{[0]} = \mathbf{B}_{[1]} \mathbf{B}_{[1]}^{\top} .$$

Hodge Laplacians

The Hodge Laplacians describe diffusion

from n-simplices to m-simplices through (m-1) and (m+1)

simplices

$$\mathbf{L}_{[m]} = \mathbf{B}_{[m]}^{\top}\mathbf{B}_{[m]} + \mathbf{B}_{[m+1]}\mathbf{B}_{[m+1]}^{\top}.$$

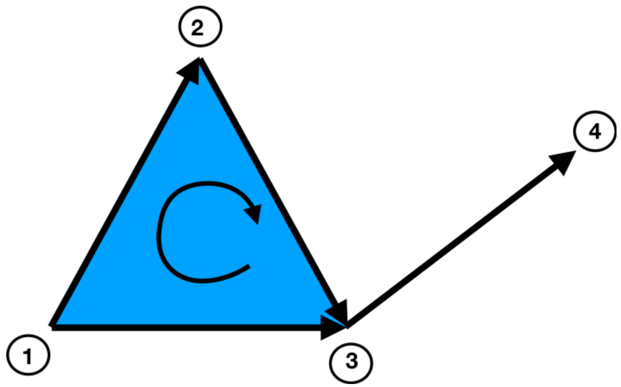
The higher order Hodge Laplacian can be decomposed as

$$\mathbf{L}_{[m]} = \mathbf{L}_{[m]}^{down} + \mathbf{L}_{[m]}^{up},$$

with

$$\mathbf{L}_{[m]}^{down} = \mathbf{B}_{[m]}^{\top}\mathbf{B}_{[m]},$$
$$\mathbf{L}_{[m]}^{up} = \mathbf{B}_{[m+1]}\mathbf{B}_{[m+1]}^{\top}.$$

Simplicial complexes and Hodge Laplacians



Hodge Laplacians

The Hodge Laplacians describe diffusion

from m-simplices to m-simplices through (m-1) and (m+1) simplices

For a 2-dimensional simplicial complex we have

$$\mathbf{L}_{[0]} = \mathbf{B}_{[1]}\mathbf{B}_{[1]}^{\top} \qquad \mathbf{L}_{[1]} = \mathbf{B}_{[1]}^{\top}\mathbf{B}_{[1]} + \mathbf{B}_{[2]}\mathbf{B}_{[2]}^{\top} \qquad \mathbf{L}_{[2]} = \mathbf{B}_{[2]}^{\top}\mathbf{B}_{[2]}$$

Properties of the Hodge Laplacians

- The Hodge Laplacians $L_m, L_m^{up}, L_m^{down}$ are semidefinite positive.
- They obey Hodge decomposition
- The dimension of the kernel of the Hodge Laplacian L_m is the m-Betti number β_m

The Hodge-Laplacians are semi-definitive positive

The Hodge Laplacians $L_m, L_m^{up}, L_m^{down}$

are semidefinite positive.

Indeed we have:

$$\langle f, L_m^{up} f\rangle = \langle f, \delta_m^* \delta_m f\rangle = \langle \delta_m f, \delta_m f\rangle \geq 0$$

$$\langle f, L_m^{down} f\rangle = \langle f, \delta_{m-1} \delta_{m-1}^* f\rangle = \langle \delta_{m-1}^* f, \delta_{m-1}^* f\rangle \geq 0$$

$$\langle f, L_m f\rangle = \langle f, L_m^{up} f\rangle + \langle f, L_m^{down} f\rangle \geq 0$$

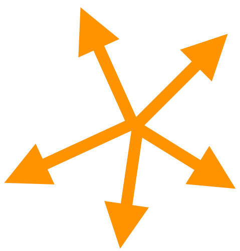
Hodge decomposition

The Hodge decomposition implies that topological signals can be decomposed

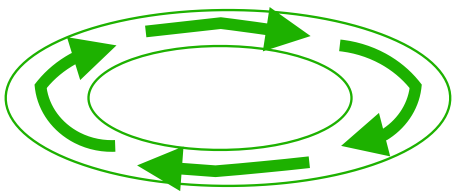
in a irrotational, harmonic and solenoidal components

$$C^m = \mathbf{im}(\mathbf{B}_{[m]}^\top) \oplus \mathbf{ker}(\mathbf{L}_{[m]}) \oplus \mathbf{im}(\mathbf{B}_{[m+1]})$$

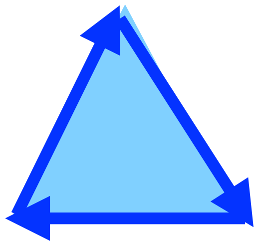
which in the case of topological signals of the links can be sketched as



Irrotational component
Gradient Flow



Harmonic component



Solenoidal component
Curl Flow

Hodge-decomposition

Given that $\mathbf{B}_{[m]}\mathbf{B}_{[m+1]} = \mathbf{0} \quad \mathbf{B}_{[m-1]}^{\top}\mathbf{B}_{[m]}^{\top} = \mathbf{0}$

and that $\mathbf{L}_{[m]}^{up} = \mathbf{B}_{[m+1]}\mathbf{B}_{[m+1]}^{\top}, \quad \mathbf{L}_{[m]}^{down} = \mathbf{B}_{[m]}^{\top}\mathbf{B}_{[m]}$

We have:

$$\mathbf{L}_{[m]}^{down}\mathbf{L}_{[m]}^{up} = \mathbf{0} \qquad \text{im}\mathbf{L}_{[m]}^{up} \subseteq \text{ker}\mathbf{L}_{[m]}^{down}$$

$$\mathbf{L}_{[m]}^{up}\mathbf{L}_{[m]}^{down} = \mathbf{0} \qquad \text{im}\mathbf{L}_{[m]}^{down} \subseteq \text{ker}\mathbf{L}_{[m]}^{up}$$

Hodge decomposition

Every m-cochain (topological signal) can be decomposed in a unique way thanks to the Hodge decomposition as

$$\mathbb{R}^{D_m} = \text{im}(\mathbf{B}_{[m]}^{\top}) \oplus \text{ker}(\mathbf{L}_{[m]}) \oplus \text{im}(\mathbf{B}_{[m+1]})$$

therefore every m-cochain can be decomposed in a unique way as

$$\mathbf{x} = \mathbf{x}^{[1]} + \mathbf{x}^{[2]} + \mathbf{x}^{harm}$$

With

$$\mathbf{x}^{[1]} = \mathbf{L}_{[m]}^{up}\mathbf{L}_{[m]}^{up,+}\mathbf{x}$$

$$\mathbf{x}^{[2]} = \mathbf{L}_{[m]}^{down}\mathbf{L}_{[m]}^{down,+}\mathbf{x}$$

Hodge decomposition

The Hodge decomposition can be summarised as

$$C^m = \textbf{im}(\mathbf{B}_{[m]}^\top) \oplus \textbf{ker}(\mathbf{L}_{[m]}) \oplus \textbf{im}(\mathbf{B}_{[m+1]})$$

This means that $\mathbf{L}_{[m]}, \mathbf{L}_{[m]}^{up}, \mathbf{L}_{[m]}^{down}$ are commuting and can be diagonalised simultaneously. In this basis these matrices have the block structure

$$\mathbf{U}^{-1}\mathbf{L}_{[m]}\mathbf{U} = \begin{pmatrix} \mathbf{D}_{[m]}^{down} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{D}_{[m]}^{up} \end{pmatrix} \quad \mathbf{U}^{-1}\mathbf{L}_{[m]}^{down}\mathbf{U} = \begin{pmatrix} \mathbf{D}_{[m]}^{down} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \end{pmatrix} \quad \mathbf{U}^{-1}\mathbf{L}_{[m]}^{up}\mathbf{U} = \begin{pmatrix} \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{D}_{[m]}^{up} \end{pmatrix}$$

- **Therefore an eigenvector in the ker of $\mathbf{L}_{[m]}$ is also in the ker of both $\mathbf{L}_{[m]}^{up}, \mathbf{L}_{[m]}^{down}$**
- **An eigenvector corresponding to an non-zero eigenvalue of $\mathbf{L}_{[m]}$ is either a non-zero eigenvector of $\mathbf{L}_{[m]}^{up}$ or a non-zero eigenvector of $\mathbf{L}_{[m]}^{down}$**

Betti numbers

The dimension of the kernel of the Hodge Laplacian L_m is the m-Betti number β_m

Indeed, thanks to Hodge decomposition

$$\begin{aligned}
\text{dim ker } \mathbf{L}_{[m]} &= \text{dim(ker } \mathbf{L}_{[m]}^{up} \cap \text{ ker } \mathbf{L}_{[m]}^{down}) \\
&= \text{dim(ker } \mathbf{L}_{[m]}^{up}) - \text{dim(im } \mathbf{L}_{[m]}^{down}) \\
&= \text{dim(ker } \mathbf{L}_{[m]}^{down}) - \text{dim(im } \mathbf{L}_{[m]}^{up}) \\
&= \text{dim(ker } \mathbf{B}_{[m]}) - \text{dim(im } \mathbf{B}_{[m+1]}) \\
&= \text{rank} \mathscr{H}_m = \beta_m
\end{aligned}$$

Expression of the matrix elements of the Hodge Laplacians

$$\mathbf{L}_m^{\text{up}}(r,s) = \begin{cases} k_{m+1,m}(\alpha_r^m), & r = s. \\ -1, & r \neq s, \alpha_r^m \frown \alpha_s^m, \alpha_r^m \sim \alpha_s^m. \\ 1, & r \neq s, \alpha_r^m \frown \alpha_s^m, \alpha_r^m \nsim \alpha_s^m. \\ 0, & \text{otherwise.} \end{cases}$$

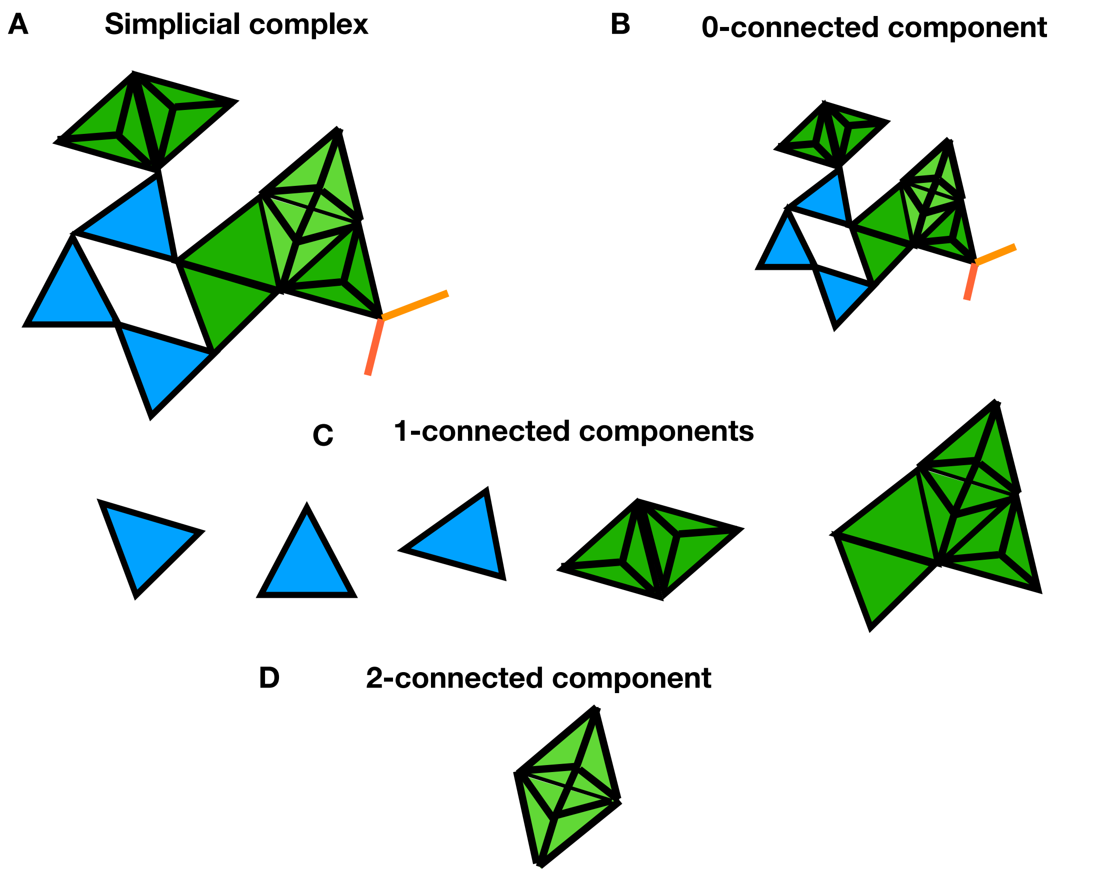
$$\mathbf{L}_m^{\text{down}}(r,s) = \begin{cases} m+1, & r = s. \\ 1, & r \neq s, \alpha_r^p \smile \alpha_s^m, \alpha_r^m \sim \alpha_s^m. \\ -1, & r \neq s, \alpha_r^p \smile \alpha_s^m, \alpha_r^p \nsim \alpha_s^m. \\ 0, & \text{otherwise.} \end{cases}$$

The m-dimensional up- Hodge Laplacian has nonzero elements only among upper incident m-simplices (simplices which are faces of a common m+1 simplex) The eigenvectors have support on the m-connected components

The m-dimensional down-Hodge Laplacian has nonzero elements only among lower incident m-simplices (simplifies sharing a m-1 face) The eigenvectors have support on the (m-1)—connected components

Here ~ indicates similar orientation with respect to the lower-simplices

m-connected components



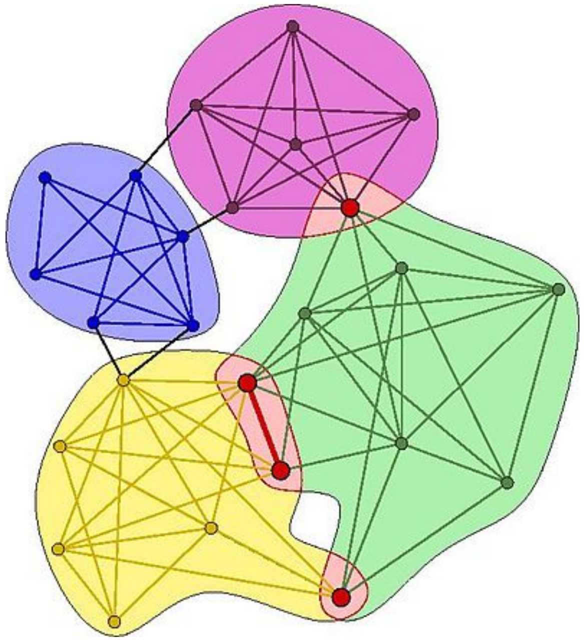
Expression of the matrix elements of the Hodge Laplacians

$$\mathbf{L}_m(r,s) = \begin{cases} k_{m+1,m}(\alpha_r^m) + m + 1, & r = s. \\ 1, & r \neq s, \alpha_r^m \not\frown \alpha_s^m, \alpha_r^m \smile \alpha_s^m, \alpha_r^m \sim \alpha_s^m. \\ -1, & r \neq s, \alpha_r^m \not\frown \alpha_s^m, \alpha_r^m \smile \alpha_s^m, \alpha_r^m \nsim \alpha_s^m. \\ 0 & \text{otherwise.} \end{cases}$$

for $0 < m < d$

The matrix elements of the Hodge Laplacian is only non zero among lower adjacent simplices that are not upper-adjacent

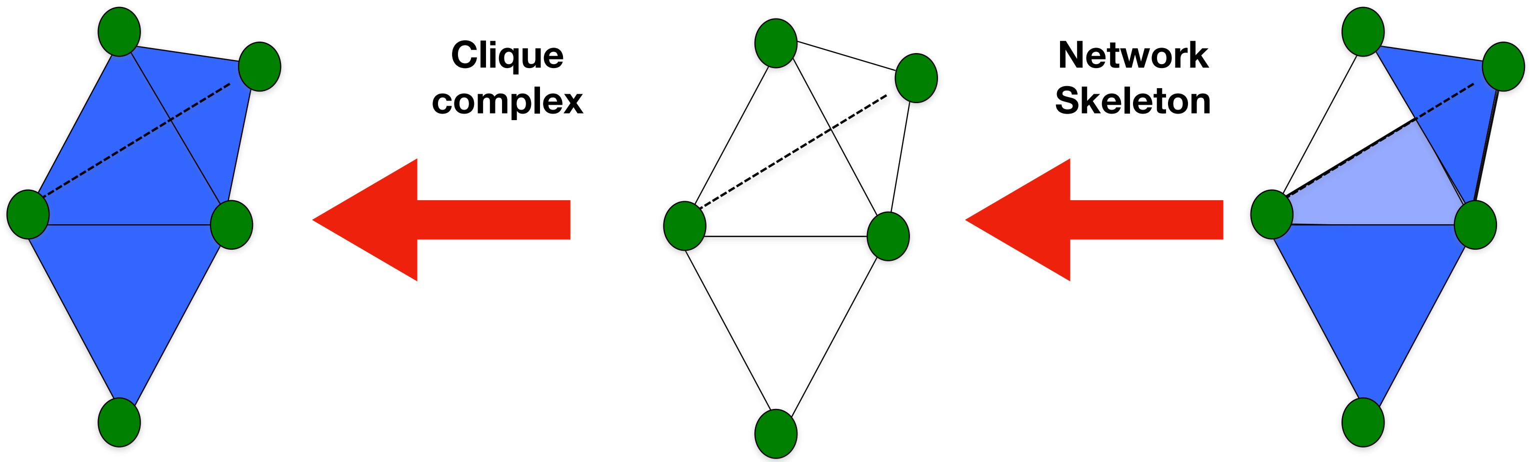
Clique communities



Palla et al. Nature 2005

The m-clique communities are the m-connected components of the clique complex of the network

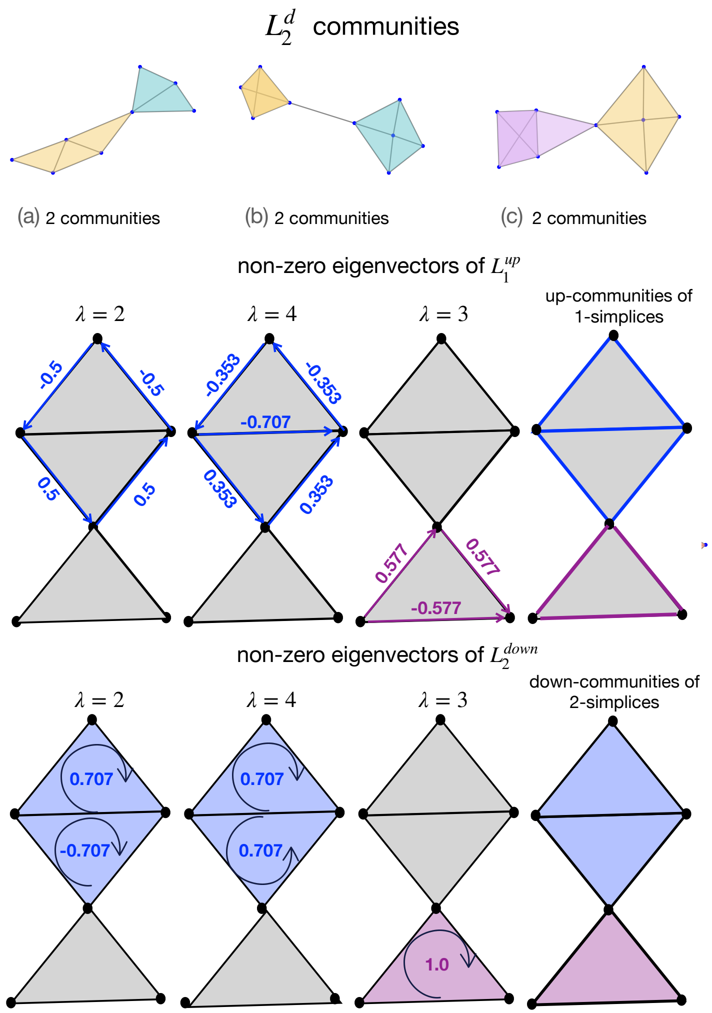
The skeleton of a simplicial complex and its clique complex



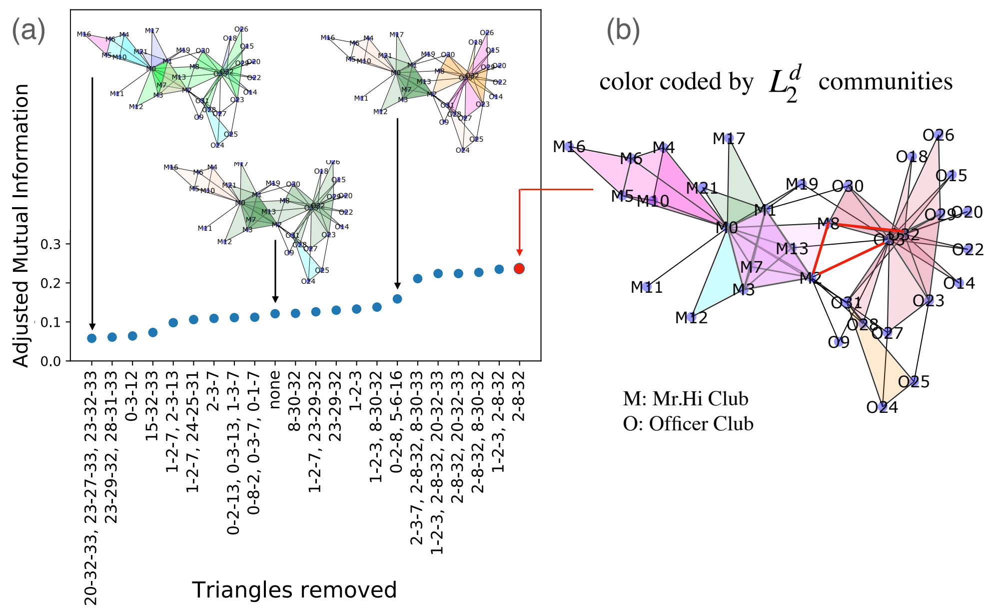
Attention!

By concatenating the operations you are not guaranteed to return to the initial simplicial complex

Higher-order communities



Inference of higher-order interactions



We can infer which higher-order interactions using higher-order communities and ground-truth community assignments

S. Khrisnagopal and GB (2021)

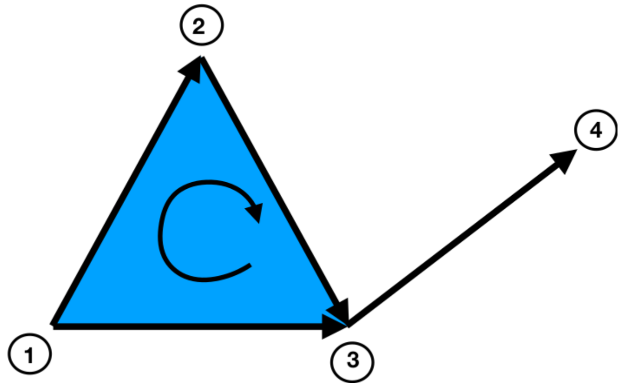
Lesson I:
Introduction to Algebraic Topology

- **Introduction to algebraic topology**

- **Higher-order operators and their properties**

1. **Topological signals**
2. **Chains and Co-chains**
3. **The boundary and the co-boundary operator**
4. **The Hodge Laplacian and Hodge decomposition**

Boundary Operators



Boundary operators

$$\mathbf{B}_{[1]} = \begin{array}{c|cccc} & [1,2] & [1,3] & [2,3] & [3,4] \\ \hline [1] & -1 & -1 & 0 & 0 \\ [2] & 1 & 0 & -1 & 0 \\ [3] & 0 & 1 & 1 & -1 \\ [4] & 0 & 0 & 0 & 1 \end{array}, \qquad \mathbf{B}_{[2]} = \begin{array}{c|c} & [1,2,3] \\ \hline [1,2] & 1 \\ [1,3] & -1 \\ [2,3] & 1 \\ [3,4] & 0 \end{array}.$$

$\mathbf{B}_{[1]}$ **Discrete divergence**

$\mathbf{B}_{[1]}^{\top}$ **Discrete gradient**

$\mathbf{B}_{[2]}^{\top}$ **Discrete Curl**

The boundary of the boundary is null

$$\mathbf{B}_{[m-1]}\mathbf{B}_{[m]} = \mathbf{0}, \quad \mathbf{B}_{[m]}^{\top}\mathbf{B}_{[m-1]}^{\top} = \mathbf{0}$$