Topology, geometry and dynamics of higher-order networks

An introduction to simplicial complexes Lesson I

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Networks



Simple network

Higher-order networks



Simplicial complex

Higher order network



Collaboration network

Higher-order brain networks



Simplicial complexes

Simplicial complexes are characterising the interactions between two ore more nodes and are formed by nodes, links, triangles, tetrahedra etc. They have been widely studied in discrete quantum gravity approaches They allow for topological and geometrical interpretation of higherorder interactions



d=2 simplicial complex



d=3 simplicial complex

Topology of Biomolecules



Topology of higher-order brain networks



Petri et al. "Homological scaffolds of brain functional networks." Journal of the Royal Society Interface 2014





Reimann et al. Cliques of neurons bound into cavities provide a missing link between structure and function. Frontiers in Computational Neuroscience 2017

Sizemore et al. Cliques and cavities in the human connectome Journal of Computational Neuroscience 2018

Higher-order networks



Network theory of higher-order networks

Providing a general view of the interplay between topology and dynamics



Higher-order structure and dynamics



Higher-order structure and dynamics



What Is Topology?





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

Can we learn the dynamics from the complex system topology?

Can we learn the topology from the complex system dynamics?

Kigher-order interactions Topology

Outline of the course:

- **1. Introduction to Homology and Cohomology**
- 2. Hodge Laplacian and Introduction to Synchronization
- 3. Topological Kuramoto model
- 4. Weighted homology and Global topological synchronization
- 5. Dirac operator and dynamics

Lesson I: Introduction to Algebraic Topology

- Introduction to simplicial complexes
- Introduction to algebraic topology
- Higher-order operators and their properties
 - 1. Topological signals
 - 2. Homology and boundary operators
 - 3. Cohomology and coboundary operators

Introduction to Simplicial complexes



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. $\alpha' \subset \alpha$.



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}

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

Dimension of a simplicial complex

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



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 ddimensional 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

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

Example

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



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 .



[Bianconi & Rahmede 2015, Courtney & Bianconi 2016]

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]





Higher-order structure and dynamics



Introduction to Algebraic Topology

Betti numbers



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)

Take Home Message: Boundary Operators



						[1,2,3]
	[1,2]	[1,3]	[2,3]	[3,4]	[1,2]	1
[1]	-1	-1	0	0	$\mathbf{B}_{[2]} = [1,3]$	-1.
$\mathbf{B}_{[1]} = [2]$	1	0	-1	0,	[2,3]	1
[3]	0	1	1	-1	[3,4]	0
[4]	0	0	0	1	L- / J	-



The boundary of the boundary is null

Boundary operators

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

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

associated to an orientation wuch that

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

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

with coefficients in \mathbb{Z} .

m-chain $c_m \in C_m$

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

Oriented simplicial complex and m-chains



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

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

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

Therefore we have







Boundary operator

THE BOUNDARY MAP

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

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

Special groups

 $\begin{aligned} & \textbf{Boundary group } \hat{B}_m = \textbf{im}(\partial_{m+1}) \\ & \textbf{Cycle group } \hat{Z}_m = \textbf{ker}(\partial_m) \end{aligned}$

The boundary of a boundary is null

The boundary operator has the property

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

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 pth missing vertex we have

$$\begin{split} \partial_{m-1}\partial_m[v_0, v_1, \dots, v_m] &= \sum_{p=0}^m (-1)^p \partial_{m-1}[v_0, v_1, \dots \hat{v}_p \dots v_m] \\ &= \sum_{p=0}^m (-1)^p \sum_{p'=0}^{p-1} (-1)^{p'} [v_0, v_1, \dots \hat{v}_{p'} \dots \hat{v}_p \dots v_m] \\ &+ \sum_{p=0}^m (-1)^p \sum_{p'=p+1}^m (-1)^{p'-1} [v_0, v_1, \dots \hat{v}_p \dots \hat{v}_{p'} \dots v_m] = 0 \end{split}$$

Incidence matrices

Given a basis for the m simplices and m-1 simplices the m-boundary operator $\partial_m[v_0, v_1, \dots, v_m] = \sum (-1)^p[v_0, v_1, \dots, v_{p-1}, v_{p+1}, \dots, v_m].$ p=0is captured by the $N_{m-1} \times N_m$ incidence (or boundary) matrix $\mathbf{B}_{[m]}$ [1,2] [1,3] [2,3] [3,4](2) [1,2,3] 1 [1,2] 3 (1) $\mathbf{B}_{[2]} = [1,3] - 1$. [2,3] 1 [3,4] 0

Boundary of the boundary is null

In terms of the incidence matrices the relation

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

Can be expressed as

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

Homology groups

THE HOMOLOGY GROUPS

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

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

denoting homology classes of *m*-cyclic chains that are in the ker(∂_m) and they do differ by cyclic chains that are not boundaries of (m + 1)-chains, i.e. they are in im(∂_{m+1}).

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

Homology



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

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

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

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.

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

Betti number



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.

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

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

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

Boundary Operators



	Boundary operators						
				-		[1,2,3]	
	[1,2]	[1,3]	[2,3]	[3,4]	[1,2]	1	
[1]	-1	-1	0	0	$\mathbf{B}_{[2]} = [1,3]$	-1.	
$\mathbf{B}_{[1]} = [2]$	1	0	-1	0,	[2,3]	1	
[3]	0	1	1	-1	[3,4]	0	
[4]	0	0	0	1			

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







Topological clustering

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



ρ	0.02 ± 0.05	0.05 ± 0.05	0.1 ± 0.05	0.15 ± 0.05	0.2 ± 0.05	
	n=120, ρ =0.014 β_0 =17, β_1 =0	n=106, ρ =0 β_0 =106, β_1 =0	n=108, ρ =0.093 $\hat{\beta}_{0}$ =1, $\hat{\beta}_{1}$ =0	n=108, ρ =0.093 β_0 =1, β_1 =0	n=108, ρ =0.11 β_0 =7, β_1 =6	
Notre Dame					***	
	n=104, ρ =0.027 β_0 =41, β_1 =11	n=114, ρ =0.089 β_0 =7, β_1 =7	n=98, ρ =0.19 $\beta_0=2, \beta_1=0$	n=99, β =0.089 β_0 =2, β_1 =0	n=99, ρ =0.21 β_0 =1, β_1 =0	
Google	*	*	*	*		Nc
	n=108, ρ =0.015 β_0 =49, β_1 =20	m=118, ρ =0.029 β_0 =36, β_1 =56	n=91, ρ =0.044 β_0 =21, β_1 =46	n=102, ρ =0.2 β_0 =13, β_1 =19	n=105, ρ =0.16 β_0 =26, β_1 =9	\
Slashdot				Mark 1		VV I
					P	of
	n=103, μ =0.0053 β_0 =83, β_1 =5	m=102, ρ =0.064 β_0 =24, β_1 =7	n=119, ρ =0.11 β_0 =9, β_1 =9	n=95, ρ =0.08 β_0 =20, β_1 =26	n=90, ρ =0.19 β_{9} =7, β_{1} =10	c a
Pokec	A		*			5a
	n=92, p=0.018	n=120, p=0.038	n=90, p=0.19	n=113, p=0.095	n=90, p=0.19	La
WikiTalk	βμ=54, β ₁ =4	β ₀ =43, β ₁ =14	β ₀ =7, β ₁ =10	β ₀ =12, β ₁ =18	β ₈ =7, β ₁ =10	di
	n=90, ρ =0.031 β_0 =1, β_1 =28					
Texan Roads	-					
	n=90, ρ =0.03 β_0 =1, β_1 =18					
Californian Roads	A.					

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

Beyond the node centered description of network dynamics The dynamical state of a simplicial complex includes node, edge, and higher-order 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						
				_	-	[1,2,3]	
	[1,2]	[1,3]	[2,3]	[3,4]	[1,2]	1	
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[4]	0	0	0	1			



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 $f : C_m \to \mathbb{R}$, that associates to every *m*-chain of the simplicial complex a value in \mathbb{R} .

m-cochain $f \in C^m$



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

Oriented simplicial complex and m-chains



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

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

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

Topological signals

Beyond the node centered description of network dynamics The dynamical state of a simplicial complex includes node, edge, and higher-order topological signals



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} .

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

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

L^2 norm between cochains

We define a scalar product between m-cochains as

 $\langle f, f \rangle = \mathbf{f}^{\mathsf{T}} \mathbf{f}$

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

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

Therefore we obtain

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

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

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Therefore we obtain

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

if follows that

$$\delta_{m+1} \circ \delta_m = 0 \ \forall m \ge 1 \text{ hence } \mathbf{B}_{[m+1]}^\top \mathbf{B}_{[m]}^\top = \mathbf{0}$$

Discrete Gradient

If $f \in C^0$, then $g = \delta_0 f \in C^1$ 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 $h = \delta_1 g \in C^2$ indicates its discrete curl

Indeed we have $\mathbf{g} = \mathbf{B}_{[2]}^{\top} \mathbf{f}$ which implies

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


Adjoint of the coboundary operator

Adjoint operator δ_m^*

The adjoint 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 adjoint 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



Boundary Operators



	Boundary operators					
				-		[1,2,3]
	[1,2]	[1,3]	[2,3]	[3,4]	[1,2]	1
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[3]	0	1	1	-1	[3,4]	0
[4]	0	0	0	1		



The boundary of the boundary is null

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