1

Lecture 13 – Higher-order networks

13a – (structure)

Apr 16, 2024

Based on: (see Canvas)

Paper 1: Siam Review 63, 3, pp. 435-485 (2021)
Paper 2: Physics Reports 874, pp. 1-92 (2020)
Paper 3: Siam Review 65, 3, pp. 686-731 (2023)
4: Siam Review 62, 2, pp. 353-391 (2020)
5: Physics Today 76, 1 pp. 36-42 (2023)

Plan:

(higher-order) "configuration models"

Opener – Slides!
Board – "boundary map", "homology"
Closing – Slides
the topology of data (pretty pictures!)
examples in neuroscience, material science, etc.
genetics, city planning, deep learning
(basically, search for "topological data analysis" on Twitter, you'll see lots of examples.)

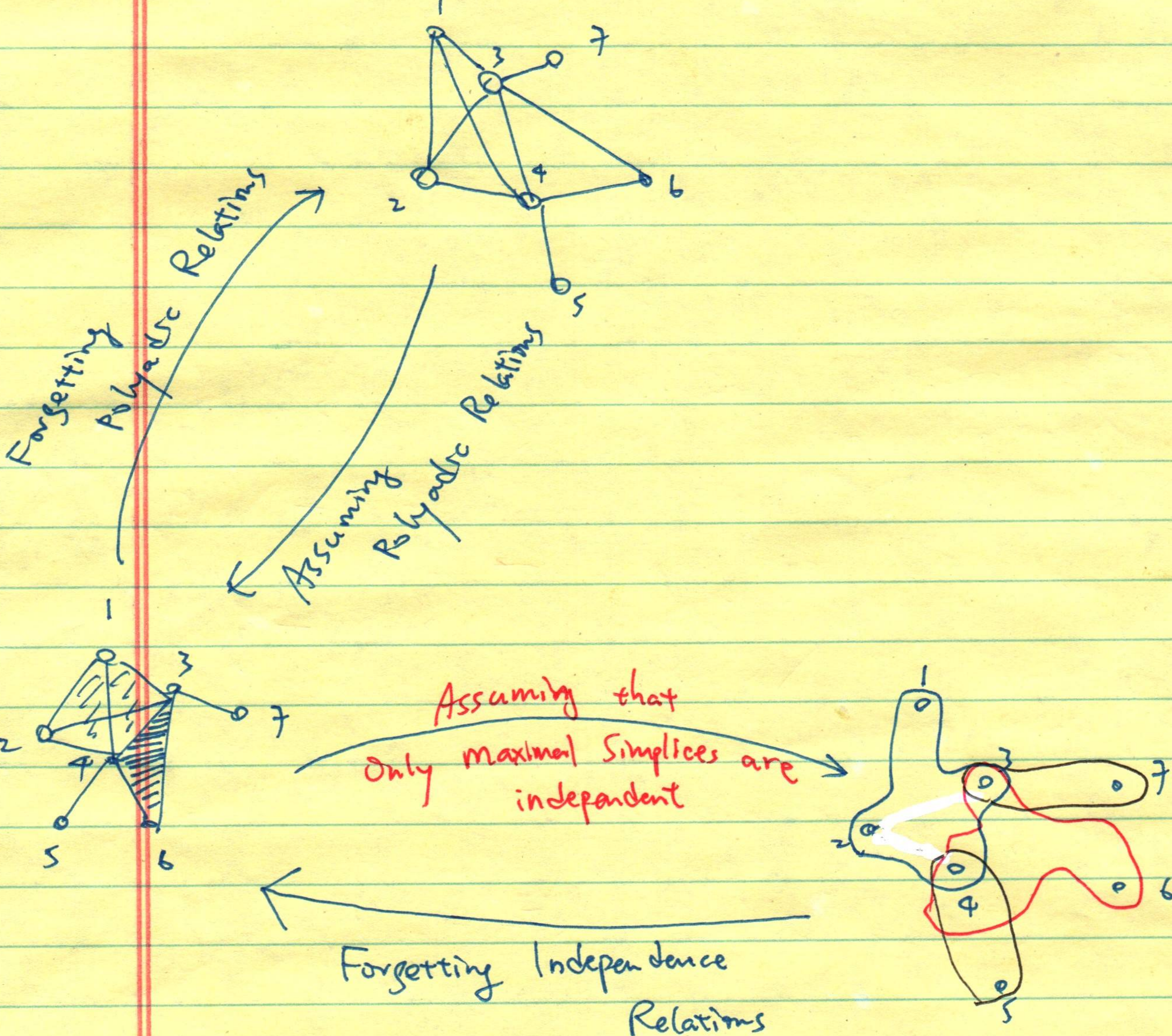
13b: dynamics

>> Hodge decomposition (think PCA)

~~>> misc topics~~

1) ~~what we missed in Lecture 11b.~~
2) ~~reconstructing a network from~~ dynamics

no time for these ...



most general !

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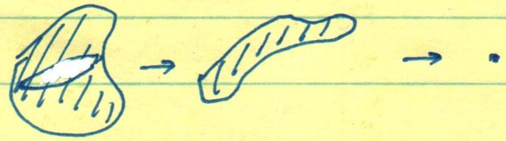
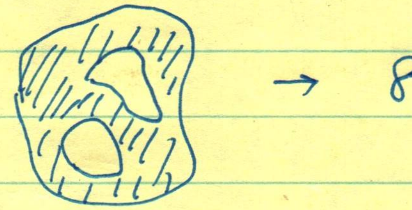
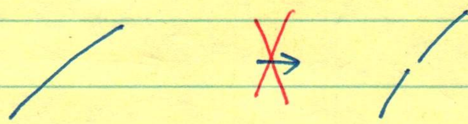
How do we formalize the idea that

1)  (same object)

2)  (same object)

3)  (different object)

$\boxed{?}$

We define the notion of " k-cycles "

- k = 3 ...
- k = 2 cavity
- k = 1 loop
- k = 0 discrete nodes

which stores the topological information we seek.

Question : When are two (k-) cycles the same ?

Answer :
>> When we can deform one cycle into the other.
>> i.e., they differ by a " filled-in cycle ", which we call the boundary of a higher-order object .

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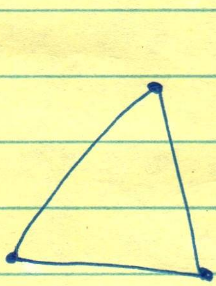
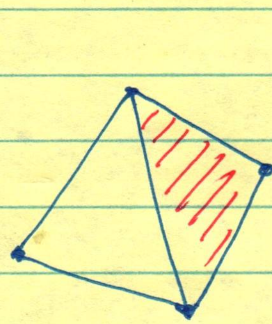
key-words : Applied topology, homological algebra, algebraic topology f.k. "computational"



1-cycle



Another 1-cycle

They are the same b/c they differ by , A 1-boundary.

» This leads to the notion of the k^{th}-homology group, which is a vector space where each basis element is a non-trivial equivalence class of k-cycles.

i.e.,

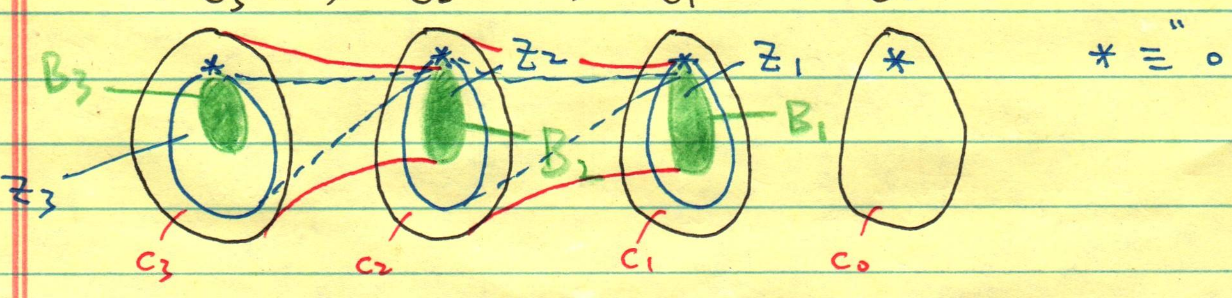
$$H_k := \underbrace{\overset{\text{cycles}}{Z_k}}_{} \Big/ \underset{\text{boundaries}}{B_k} = \frac{\ker \partial_k}{\operatorname{im} \partial_{k+1}}$$

We can mathematically formalize the idea using a ---

"chain complex" $\equiv (C_\bullet, \partial_\bullet)$ $\quad \partial_k : C_k \to C_{k-1}$

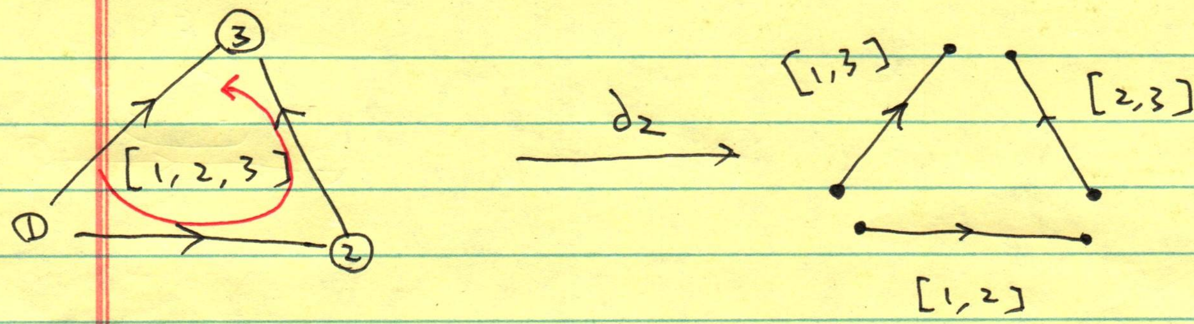
$$\boxed{\begin{aligned} \ker(\partial_k) &= Z_k \\ \operatorname{im}(\partial_k) &= B_{k-1} \end{aligned}}$$

$$\cdots \to C_3 \xrightarrow{\partial_3} C_2 \xrightarrow{\partial_2} C_1 \xrightarrow{\partial_1} C_0 \to 0$$



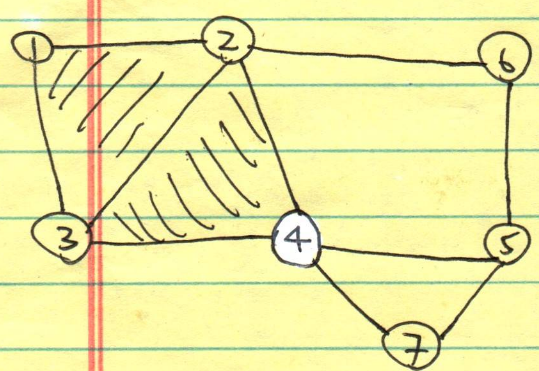
Paper 4.
Siam Review 62, 2
pp. 353-391

"Help! This is way too abstract!"



$$[1,2,3] \xrightarrow{\partial_2} [2,3] - [1,3] + [1,2]$$

{ Steps to create boundary maps.



1) Identify the basis elements

0-chain : node id's

1-chain : [1,2]
[1,3]
[2,3]
⋮
[5,7]

when doing so, we also fix the orientation.

2-chain : [1,2,3]
[2,3,4]

again, "orientation" is fixed.

$|C_2| = 2$

$|C_1| = 6$

$|C_0| = 7$

orientation = increasing indices.

⑥

2) We can write down the boundary map, according to

$$\partial_k [i_0, i_1, \cdots, i_k] = \sum_{j=0}^{k} (-1)^j [i_0, \cdots, i_{j-1}, i_{j+1}, \cdots, i_k]$$

$$\mathbb{B}_1 = \begin{array}{c|ccccc} & [1,2] & [1,3] & [2,3] & [2,4] & \cdots \\ \hline 1 & -1 & -1 & 0 & 0 & \\ 2 & 1 & 0 & -1 & -1 & \\ 3 & 0 & 1 & 1 & 0 & \\ 4 & 0 & 0 & 0 & 1 & \\ 5 & 0 & 0 & 0 & 0 & \\ 6 & 0 & 0 & 0 & 0 & \\ 7 & 0 & 0 & 0 & 0 & \end{array}$$

$\mathbb{B}_1 \Rightarrow$ 7-by-10 matrix

$\mathbb{B}_2 \Rightarrow$ 10-by-2 matrix

check that

$\mathbb{B}_1 \cdot \mathbb{B}_2 = 0$

$$\mathbb{B}_2 = \begin{array}{c|cc} & [1,2,3] & [2,3,4] \\ \hline [1,2] & 1 & 0 \\ [1,3] & -1 & 0 \\ [2,3] & 1 & 1 \\ [2,4] & 0 & -1 \\ [2,6] & 0 & 0 \\ [3,4] & 0 & 1 \\ \vdots & \vdots & \vdots \end{array}$$

See Paper 4, p.381

⑦ "minimal homology basis" (see eg. Scientific Reports, 11, 5355 (2021))

⇕ related problem

Betti number : The dimension of the k-th homology group tells us the number of topoligical cavities.

i.e., $\dim(H_k) = \dim(Z_k) - \dim(B_k) \equiv \beta_k$

Where can we obtain β_k ? Ans : In the matrix expression of ∂_k & ∂_{k+1} !

∂_k or $\mathbb{B}_k$ in "Smith's normal form"

$$\begin{array}{ccc} & & \leftarrow \text{rank } Z_k \rightarrow \\ \text{rank } B_{k-1} & \left[\begin{array}{c|c} \begin{matrix} 1 & & 0 \\ & \ddots & \\ 0 & & 1 \end{matrix} & 0 \\ \hline 0 & 0 \end{array}\right] & \text{rank } C_{k-1} \\ & \leftarrow \text{rank } C_k \rightarrow & \end{array}$$

$\beta_k = \text{rank}(Z_k) - \text{rank}(B_k)$

Summary

1) $\{\partial_k\}$ "filtration" or $\{\mathbb{B}_k\}$ contain key topological information !

2) $\{\mathbb{B}_k^{(t)}\}$ defines an idea of "persistent homology" (see slides !)

"persistent homology" $\in$ { toolbox of topological data analysis }.

Next Lecture !

3) $\{\mathbb{B}_k\}$ allow us to define "combinatorial Hodge Laplacian"

3.1) Generalization of the graph Laplacian.

3.2) Through "Hodge decomposition" — A powerful tool in (topological) signal processing.

①

or (Signal processing on graphs and high-order networks)

136 - dynamics

Apr 18, 2024

Today's lecture adds three more papers to the reference.

Paper 6 : Proceedings of the IEEE, 106, 5, pp. 808-828 (2018)

7 : Signal Processing, 187, 108149 (2021)

8 : J. Royal Society Interface 19: 20220043 (2022)

Review :

Tue. we introduced "boundary maps", they are useful for

- computing the Betti numbers
- computing the "persistent homology"
- computing the (k-th) combinatorial Hodge Laplacian.

Today, we will

- walk thru the (unfinished) example from Tues.
- define the Hodge Laplacians / learn their properties.
- slides (from Papers 4, 5, 6, 7)

k-th combinatorial Hodge Laplacian

Primer : graph Laplacian

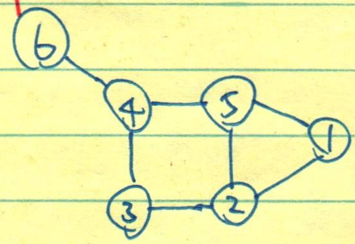
Given simple graph $G = (V, E)$, where $|V| = n$, its Laplacian matrix $L_{n \times n}$ is defined element-wise as

$$L_{ij} = \begin{cases} \deg(v_i) & \text{if } i = j \\ -1 & \text{if } i \neq j \text{ and } (v_i, v_j) \in E \\ 0 & \text{otherwise} \end{cases}$$

OR, $L \equiv \underbrace{D}_{\text{degree matrix}} - \overbrace{A}^{\text{adjacency matrix}}$

②

example :



$$L = \begin{pmatrix} 2 & -1 & & & -1 & \\ -1 & 3 & -1 & & -1 & \\ & -1 & 2 & -1 & & \\ & & -1 & 3 & -1 & -1 \\ -1 & -1 & & -1 & 3 & \\ & & & -1 & & 1 \end{pmatrix}$$

Properties of the Laplacian matrix L

» Because $V = (1, 1, \cdots, 1)$ satisfies $LV = 0$,
"zero" is one of the eigenvalues of L.

» Actually, if we order L's all eigenvalues, $\lambda_0 \le \lambda_1 \le \cdots \le \lambda_{n-1}$
$\lambda_0 = 0$

» Othogonal fact, L is "positive-semidefinte" (PSD)

Def 1 : $\lambda_i \geq 0$

2 : $x^T L x \geq 0, \ \forall x \in \mathbb{R}^n$

Let's prove this by :

→ FACT 1 : L can be written as $L = B B^T$,
where B is the incidence matrix of a digraph

$$B_{im} \begin{cases} 1 & \text{if edge } e_m \text{ enters vertex } V_i \\ -1 & \text{if edge } e_m \text{ leaves vertex } V_i \\ 0 & \text{otherwise.} \end{cases}$$

dimension = $|V| \times |E|$

Assuming $i \to j$ if
$ID(i) < ID(j)$

So... edge $(1,2)$, you'll have ① → ②

③

$$(BB^T)_{ij} = \sum_{m=1}^{|E|} B_{im} B_{jm}$$

of dimension $|V| \times |V|$ now (hence the dummy j)

$$B_{im} B_{jm} = \begin{cases} 1 & \text{if } i = j \quad \left(\text{b/c } \begin{matrix} -1 \times -1 = 1 \\ 1 \times 1 = 1 \end{matrix}\right) \\ -1 & \text{if } i \neq j \quad \left(\text{b/c } \begin{matrix} -1 \times 1 = -1 \\ 1 \times -1 = -1 \end{matrix}\right) \\ 0 & \text{otherwise.} \end{cases}$$

$$(BB^T)_{ij} = \begin{cases} D_{ii} = d_i & \\ -1 & \\ 0 & \text{otherwise} \end{cases}$$

increment by 1 whenever there's an edge incident on i

Therefore $BB^T = D - A = L$.

Now, we rewrite $x^T L x = x^T (BB^T) x$

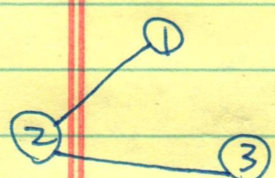
$$= (x^T B)(B^T x)$$

see example

$$= (B^T x)^T (B^T x)$$

$$= \sum_{i<j} (x_j - x_i)^2 \geq 0$$

QED.



$$\begin{array}{cc} & \begin{matrix} (1,2) & (2,3) \end{matrix} \\ B = \begin{matrix} 1 \\ 2 \\ 3 \end{matrix} & \begin{pmatrix} -1 & 0 \\ 1 & -1 \\ 0 & 1 \end{pmatrix} \end{array}$$

$$B^T x = \begin{pmatrix} -1 & 1 & 0 \\ 0 & -1 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} -x_1 + x_2 \\ -x_2 + x_3 \end{pmatrix} \Rightarrow (B^T x)^T (B^T x) = (x_2 - x_1)^2 + (x_3 - x_2)^2$$

dimension 2×3 $\quad 3 \times 1$ $\quad 2 \times 1$

④

from previous page :

Cont'd : Properties of the graph Laplacian, L

» The second smallest eigenvalue is called the algebraic connectivity of G.

Furthermore,

① its eigenvector approximates the sparsest cut (an NP-hard problem) of G.

② The number of zero eigenvalues tells you the number of connected components.

$x^T L x = \lambda$ if $x \in \mathbb{R}^n$ is a normalized eigenvector.
$\{ x^T x = 1$

The $(x_j - x_i)^2$ terms measure some "strain" along the edges connecting the nodes i, j.

» $\boxed{\text{fewer strain} \Rightarrow \text{smaller } \lambda}$

» implications in "graph signal processing"

"graph filters" signal processing on graphs

(analogy in PCA, Fourier transform, etc.)

"graph Fourier transform"

"frequency of the graph signal"

**

See Figs 3 & 4 of Paper 6
1–3 of Paper 7.

Finally, Hodge Laplacian

We are carrying the intuitions about
smothness
projection (into useful subspaces)
into higher-dimensional counterparts of the Laplacian,
called Hodge Laplacian.

Definition k^{th} combinatorial Hodge Laplacian

$$L_k = B_k^T B_k + B_{k+1} B_{k+1}^T$$

Remark because $B_0 = 0$, $L_0 = B_1 B_1^T$; that's the (combinatorial) graph Laplacian, or Hodge 0-Laplacian.
They allow you to analyze signals on the nodes !

L_1, or 1-Laplacian, allow you to analyze signals on the edges !

"Hodge decomposition"

we can decompose $C_k \simeq \mathbb{R}^{n_k} = \underbrace{\operatorname{im}(B_{k+1}) \oplus \operatorname{im}(B_k^T) \oplus \ker(L_k)}_{\text{useful subspaces !}}$

example :
when $k=1 \Rightarrow$ "one-dim chains"
$n_k = |E|$, C_k = set of edges

⑥

We focus on $k=1$.

curl flow

harmonic flow.

$$C_1 = \mathrm{im}\left(B_2\right) \oplus \mathrm{im}\left(B_1^T\right) \oplus \underbrace{\ker\left(L_1\right)}$$

edge flow

gradient flow

Examples, see Figs. 4.1 of Paper 4
5.2
5.3

things that, after the action of L_1,
become zero.

in our previous lecture

$\begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix}$ is an eigenvector of L_0,

therefore, $\begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix} \in \ker(L_0)$.

** We did not use figures in Papers 1, 2, 3, and 8.
BUT, they are great review papers!