Topological Data Analysis

Lecture 7
Higher-order Laplacian

Oleg Kachan

Graph Laplacian

Graph

$$G = (V, E),\ \text{where } E \subseteq V \times V\,.$$

Adjacency matrix

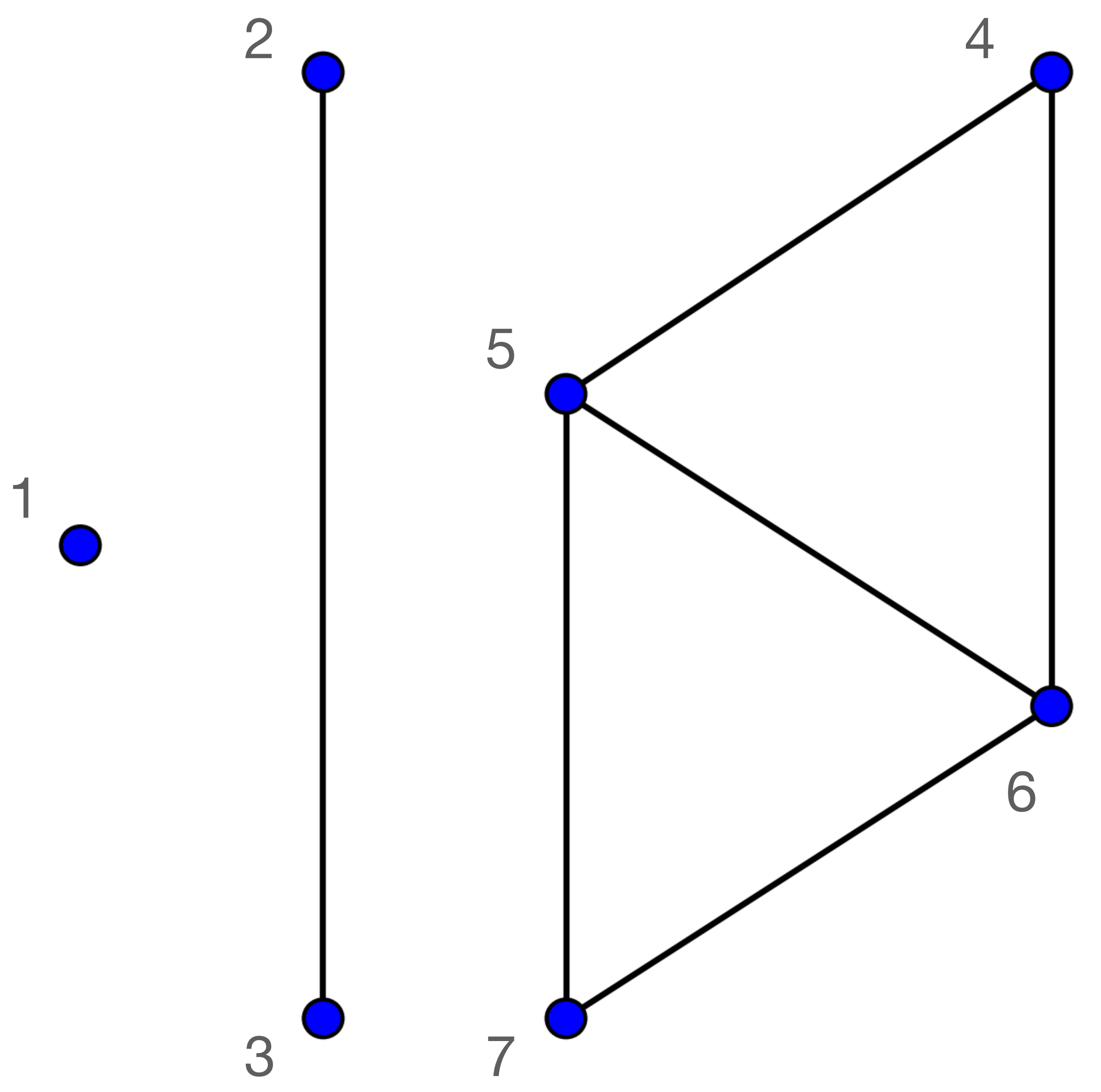
A is |V| x |V| matrix.

$$\mathbf{A}_{ij} = \begin{cases} 1, & v_i \sim v_j, \\ 0, & \text{otherwise}\,. \end{cases}$$

Incidence matrix

B is |V| x |E| matrix.

$$\mathbf{B}_{ij} = \begin{cases} 1, & v_i \sim v_j, v_i \succ v_j, \\ -1, & v_i \sim v_j, v_i \prec v_j, \\ 0, & \text{otherwise}\,. \end{cases}$$



Graph *G*

Graph Laplacian

Graph

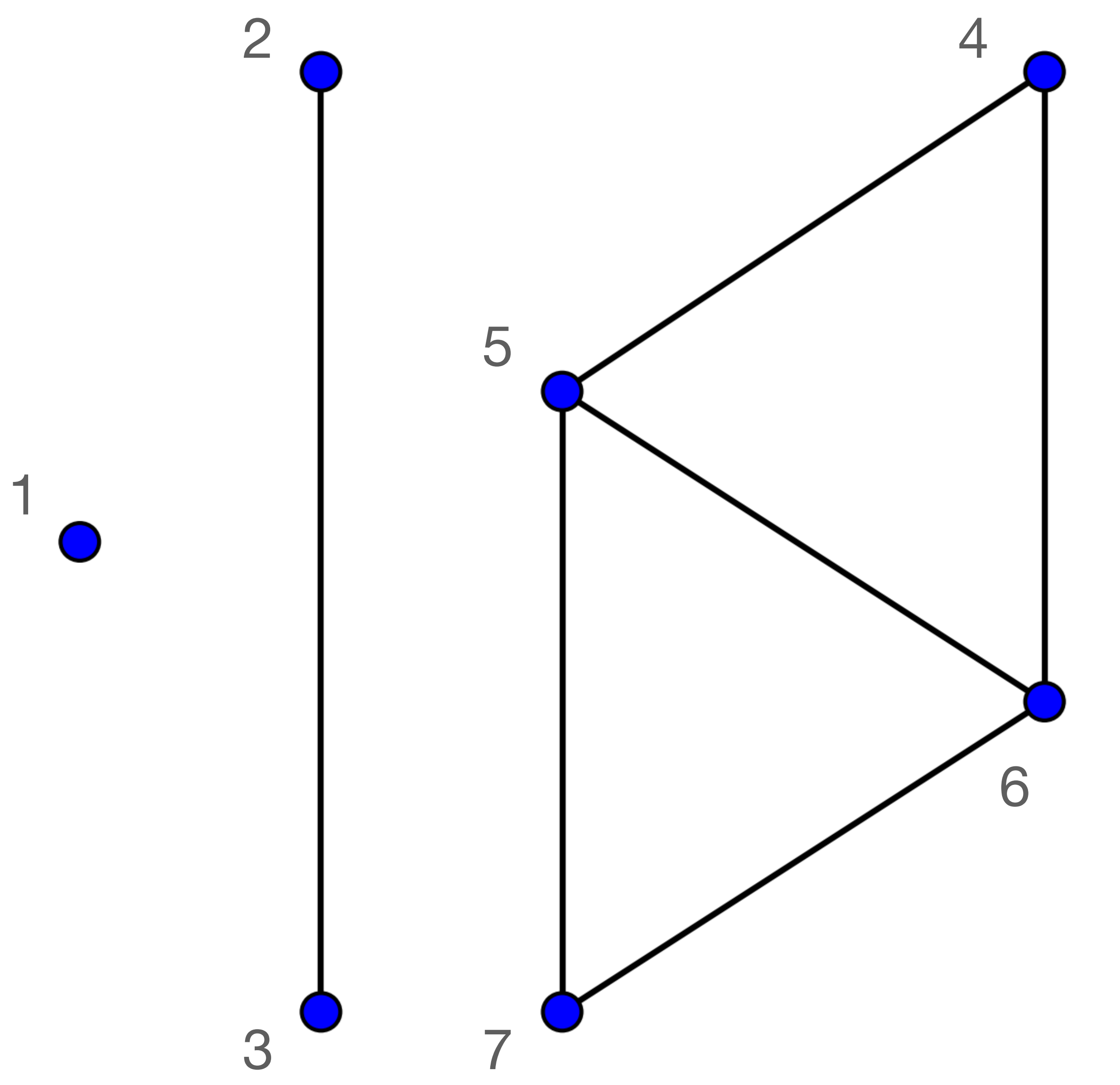
$$G = (V, E), \text{ where } E \subseteq V \times V\,.$$

Laplacian matrix

L is |V| x |V| matrix.

$$\mathbf{L}_{ij} = \begin{cases} d(v_i), & i = j, \\ -1, & i \neq j \text{ and } v_i \sim v_j, \\ 0, & \text{otherwise}\,. \end{cases}$$

	1	2	3	4	5	6	7
1	0						
2		1	-1				
3		-1	1				
4				2	-1	-1	
5				-1	3	-1	-1
6				-1	-1	3	-1
7					-1	-1	2



Graph *G*

Laplacian via adjacency

$$\mathbf{L} = \mathbf{D} - \mathbf{A}$$

Laplacian via incidence

$$\mathbf{L} = \mathbf{B}\mathbf{B}^T$$

Graph Laplacian

$$(BB^T)_{ij} = \sum_{k=1}^{n} B_{ik}B_{jk}$$

$$B_{ik}B_{jk} = \begin{cases} 1, & i = j, (i,j) \in E, \\ -1, & i \neq j, (j,i) \in E, \\ 0, & \text{overwise}\,. \end{cases} \qquad (BB^T)_{ij} = \begin{cases} \sum_{k|i \in E_k} 1, & i = j, \\ -1, & i \neq j, \\ 0, & \text{overwise}\,. \end{cases}$$

$$\sum_{k|i \in E_k} 1 = \deg(v_i)$$ *is the degree of i-th vertex, therefore* $\mathbf{B}\mathbf{B}^T = \mathbf{D} - \mathbf{A}$

Graph Laplacian

Properties

- real symmetric
- rows/columns sums to 0
- positive-semidefinite, all eigenvalues >=0, eigenvalues are real

- $\lambda_0 = 0$, as $\boldsymbol{v}_0 = (1, 1, \ldots, 1)^T$ satisfies $\boldsymbol{L}\boldsymbol{v}_0 = 0$
- the number of connected components of G is the dimension of the nullspace (kernel) of L

Higher-order Laplacian

Simplicial complex

$$K = \left(\Sigma_0, \Sigma_1, \ldots, \Sigma_{\dim(K)}\right)$$

Chain space

$$C_k = \left\{a\sigma_k \mid a \in \mathbb{F}, \sigma_k \in \Sigma_k\right\}$$

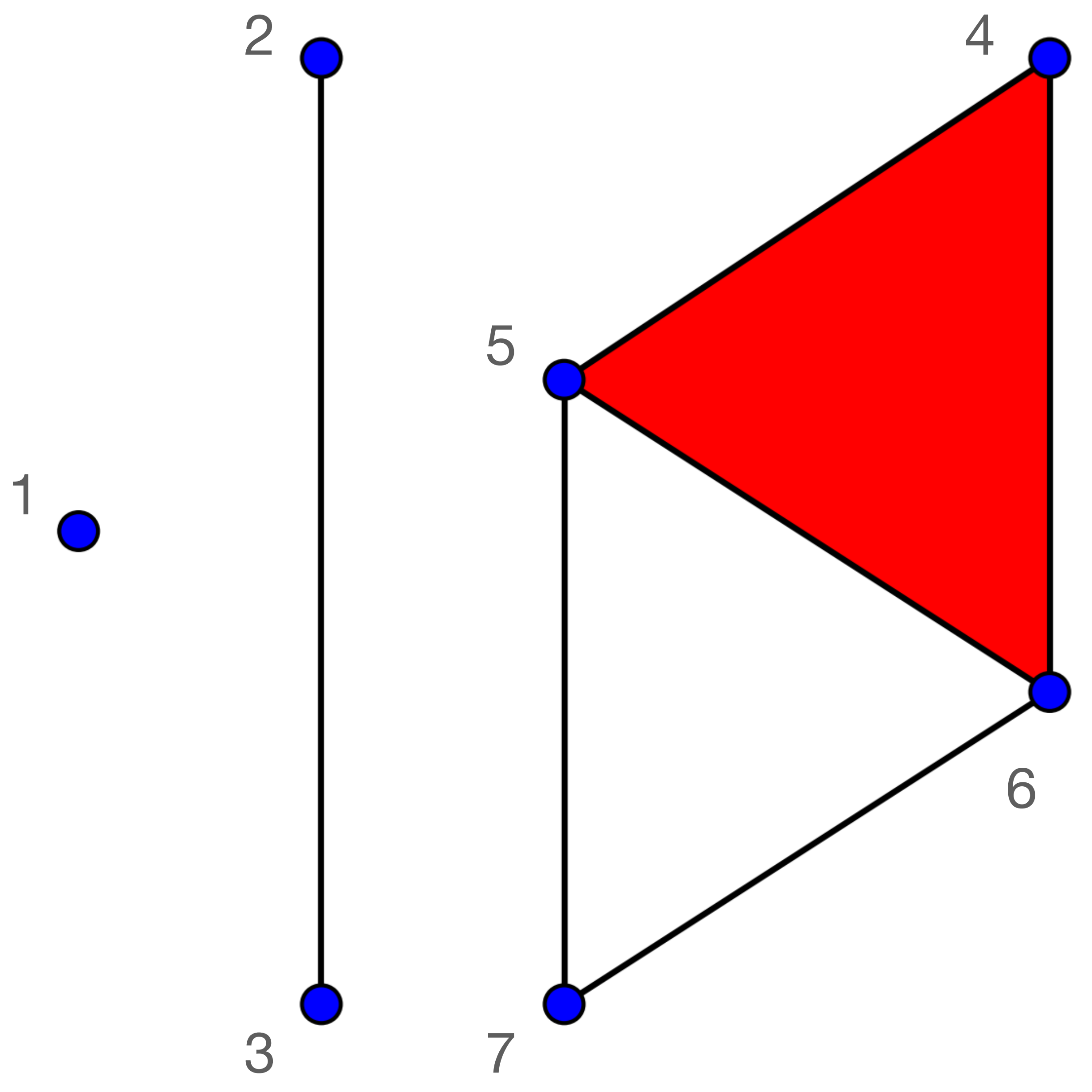
Boundary operator

$$\partial_k : C_k \to C_{k-1}$$

$$\partial_k([v_0, \ldots, v_k]) = \sum_{i=0}^{k} (-1)^i [v_0, \ldots, \hat{v}_i, \ldots, v_k]$$

$$\partial_1([2,3]) = 3 - 2$$

$$\partial_2([4,5,6]) = [5,6] - [4,6] + [4,5]$$



Simplicial complex *K*

$\mathbf{B}_1 =$

	23	45	46	56	57	67
1						
2	-1					
3	1					
4		-1	-1			
5		1		-1	-1	
6			1	1		-1
7					1	1

$\mathbf{B}_2 =$

	456
23	
45	1
46	-1
56	1
57	
67	

Higher-order Laplacian

Chain complex of *K*

$$\dots \xrightarrow{\partial_3} C_2 \xrightarrow{\partial_2} C_1 \xrightarrow{\partial_1} C_0 \xrightarrow{\partial_0} 0$$

$$\partial_k \circ \partial_{k+1} = 0$$

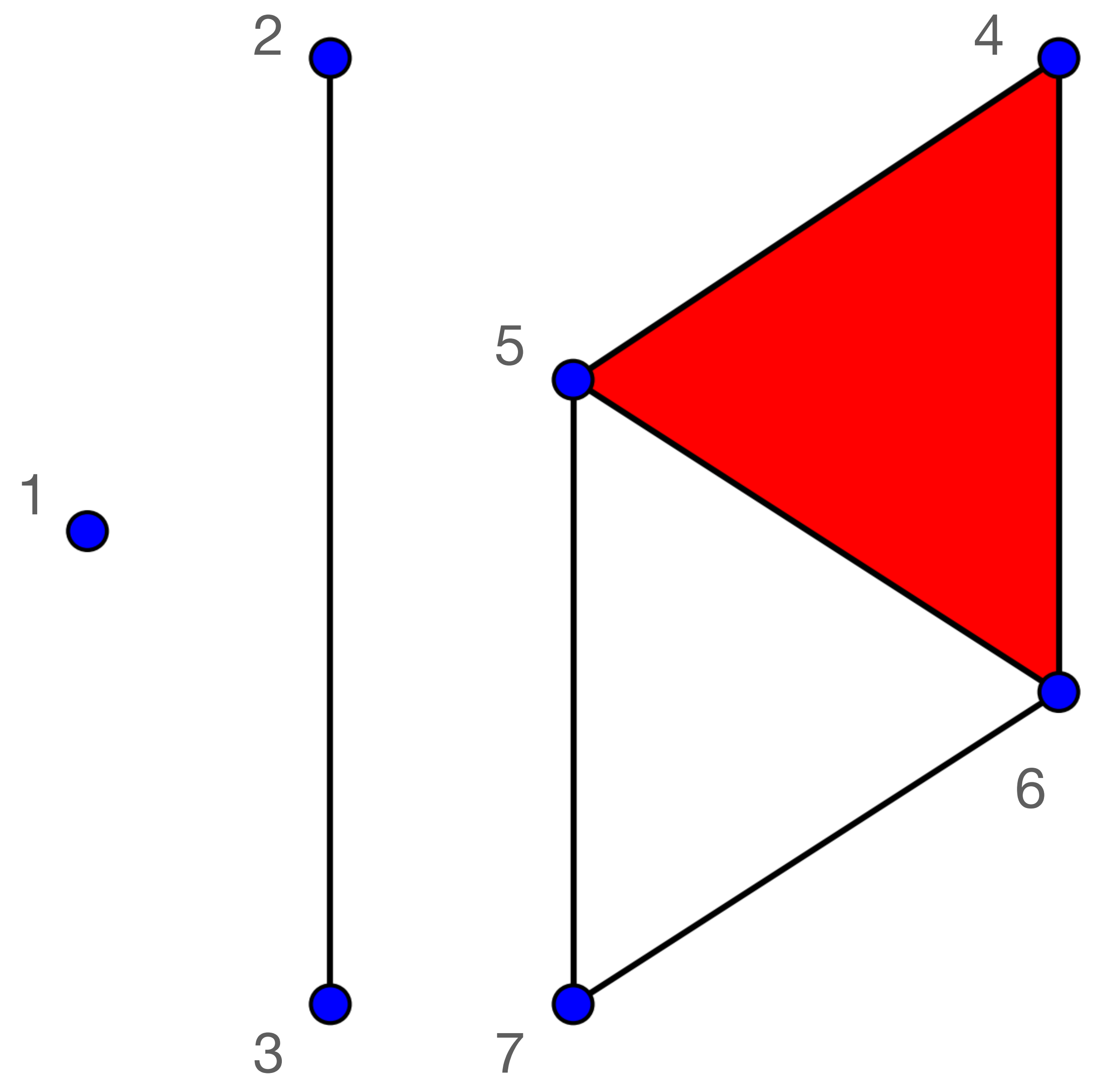
Higher-order Laplacian operator

$$L_k = \partial_k^* \partial_k + \partial_{k+1} \partial_{k+1}^*$$

Higher-order Laplacian

The multiplicity of zero eigenvalue of $\boldsymbol{L}_k$ equals the rank of the k-th homology group H_k of K.

$$\dim \ker(\mathbf{L}_k) = H_k(K)$$



Simplicial complex *K*

Generalized higher-order Laplacian

Generalized chain complex of *K*

$$
\begin{tikzcd}
C_3 \arrow[r, "\partial_{3,1}"] \arrow[rr, bend right, "\partial_{3,2}"'] \arrow[rrr, bend right=40, "\partial_{3,3}"'] & C_2 \arrow[r, "\partial_{2,1}"] \arrow[rr, bend right, "\partial_{2,2}"'] & C_1 \arrow[r, "\partial_{1,1}"] & C_0
\end{tikzcd}
$$

Generalized boundary operator

$$\partial_{k,p} : C_k \to C_{k-p}$$

$$\partial_{k,p}([v_{\eta(0)}, \ldots, v_{\eta(k)}]) = \sum_{j_1,\ldots,j_p} \mathrm{sgn}(\eta)\mathrm{sgn}(\varepsilon_{j_1\ldots j_p})[v_0, \ldots, \hat{v}_{j_1}, \ldots, \hat{v}_{j_p}, \ldots, v_k]$$

Given the (k-p)-face τ of k-simplex σ = $[v_0, \ldots, \hat{v}_{j_1}, \ldots, \hat{v}_{j_p}, \ldots, v_k]$ *denote the permutation*

$$\varepsilon_{j_1\ldots j_p} = \begin{pmatrix} 0 & \ldots & p-1 & k & \ldots & k \\ j_1 & \ldots & j_h & 1 & \ldots & 1 \end{pmatrix}$$

Simplicial Degree in Complex Networks. Applications of Topological Data Analysis to Network Science
Serrano D.H. et al. *Chaos, Solitons & Fractals (2020)*

Generalized higher-order Laplacian

Generalized chain complex of *K*

$$\begin{tikzcd} C_3 \arrow[r, "\partial_{3,1}"] \arrow[rr, bend right, "\partial_{3,2}"'] \arrow[rrr, bend right=50, "\partial_{3,3}"'] & C_2 \arrow[r, "\partial_{2,1}"] \arrow[rr, bend right, "\partial_{2,2}"'] & C_1 \arrow[r, "\partial_{1,1}"] & C_0 \end{tikzcd}$$

Generalized Laplacian operator

$$L_{k,p,q} = \partial^*_{k,p}\partial_{k,p} + \partial_{k+q,q}\partial^*_{k+q,q}$$

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Higher-order Laplacian

Spectrum

Higher-order Laplacian operator

$$\begin{tikzcd} C_2 \arrow[r, shift left, "\partial_2"] & C_1 \arrow[l, shift left, "\partial_2^*"] \arrow[r, shift left, "\partial_1"] & C_0 \arrow[l, shift left, "\partial_1^*"] \end{tikzcd}$$

$$L_k = \partial_k^* \partial_k + \partial_k \partial_k^*$$

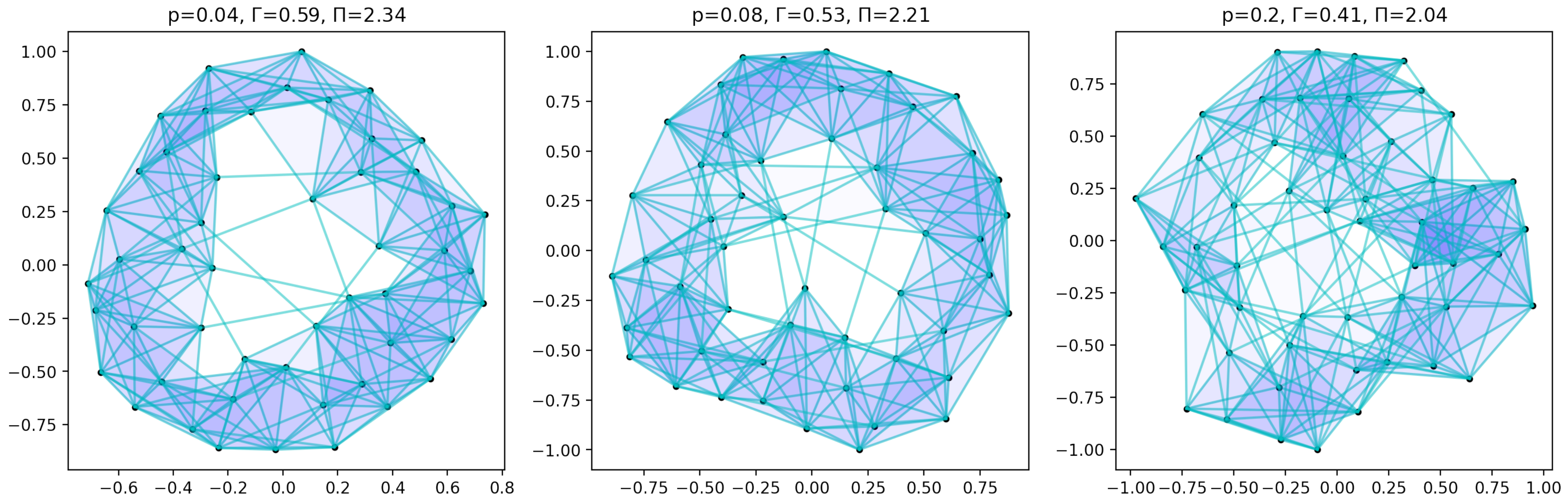
Generalized Laplacian operator

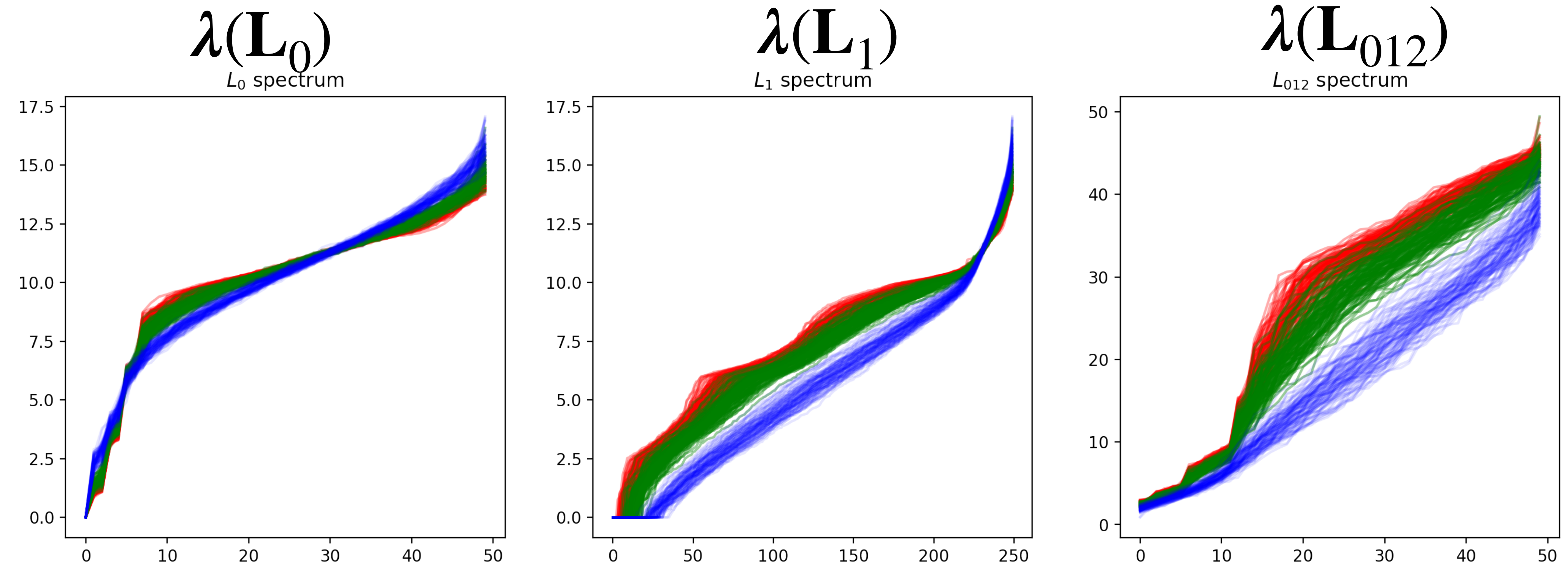
$$\begin{tikzcd} C_3 \arrow[r, "\partial_{3,1}"] \arrow[rr, bend right, "\partial_{3,2}"'] \arrow[rrr, bend right=50, "\partial_{3,3}"'] & C_2 \arrow[r, "\partial_{2,1}"] \arrow[rr, bend right, "\partial_{2,2}"'] & C_1 \arrow[r, "\partial_{1,1}"] & C_0 \end{tikzcd}$$

$$L_{k,p,q} = \partial_{k,p}^* \partial_{k,p} + \partial_{k+q,q} \partial_{k+q,q}^*$$

Watts-Strogatz model $G(n, m, p)$

$n = 35,\ m = 15,\ p = \{0.01, 0.1, 0.4\}$, 500 graphs of each class





L0	L1	L012
73.91 ± 0.86	78.37 ± 0.62	**84.08 ± 0.49**

Classification accuracy, % for 5-fold cross-validation averaged over 10 runs.

Graph Laplacian

$\dim \ker(\mathbf{L}) = \#\ \text{connected components}(G)$

$\left(0,\ (1,1,\ldots,1)^T\right)$ is eigenpair of $\mathbf{L}$.

$\mathbf{L1} = 0$

$m_i = \sum_{j=1}^{n} \ell_{ij}$

m_i is 0 for all i, at rows of L sum to 0.

Therefore 0 is the eigenvalue of ***L***.

$0 \leq \lambda_1 \leq \lambda_2 \leq \ldots \lambda_n$

$\mathbf{z}^T\mathbf{L}\mathbf{z} = \mathbf{z} \cdot 0 = 0$

$\mathbf{z}^T\mathbf{L}\mathbf{z} = \sum_{(u,v)\in E} (z_u - z_v)^2 = 0$