# Topological Data Analysis

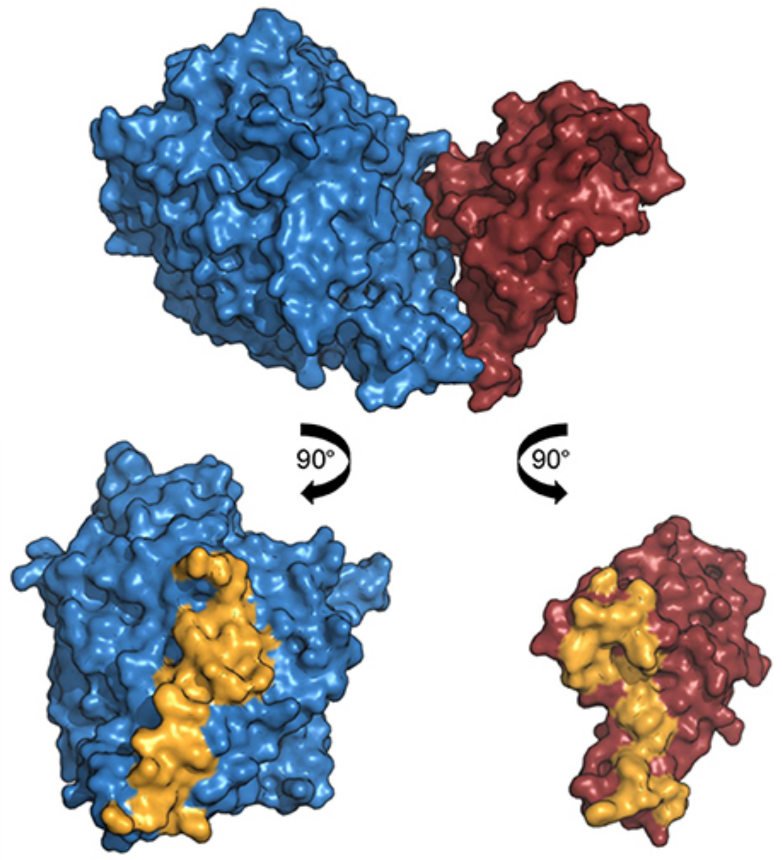
**Lecture 8**

Higher-order Network Science

**Oleg Kachan**

# Complex networks

**Social and collaboration networks**




**Protein interaction networks**

**Functional brain networks**

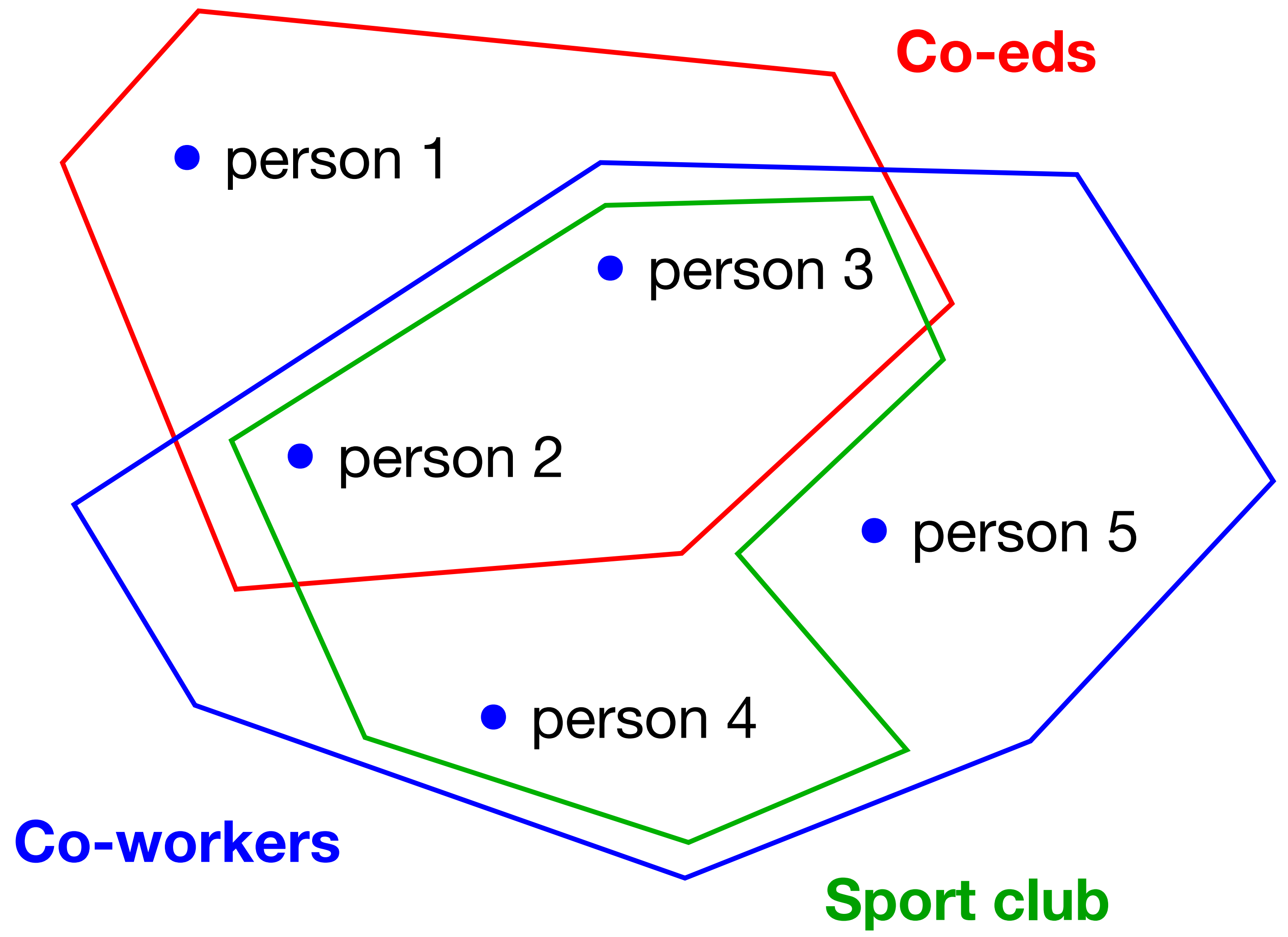

**Financial networks**

Networks Beyond Pairwise Interactions: Structure and Dynamics
Battiston et al. *Physics Reports (2020)*

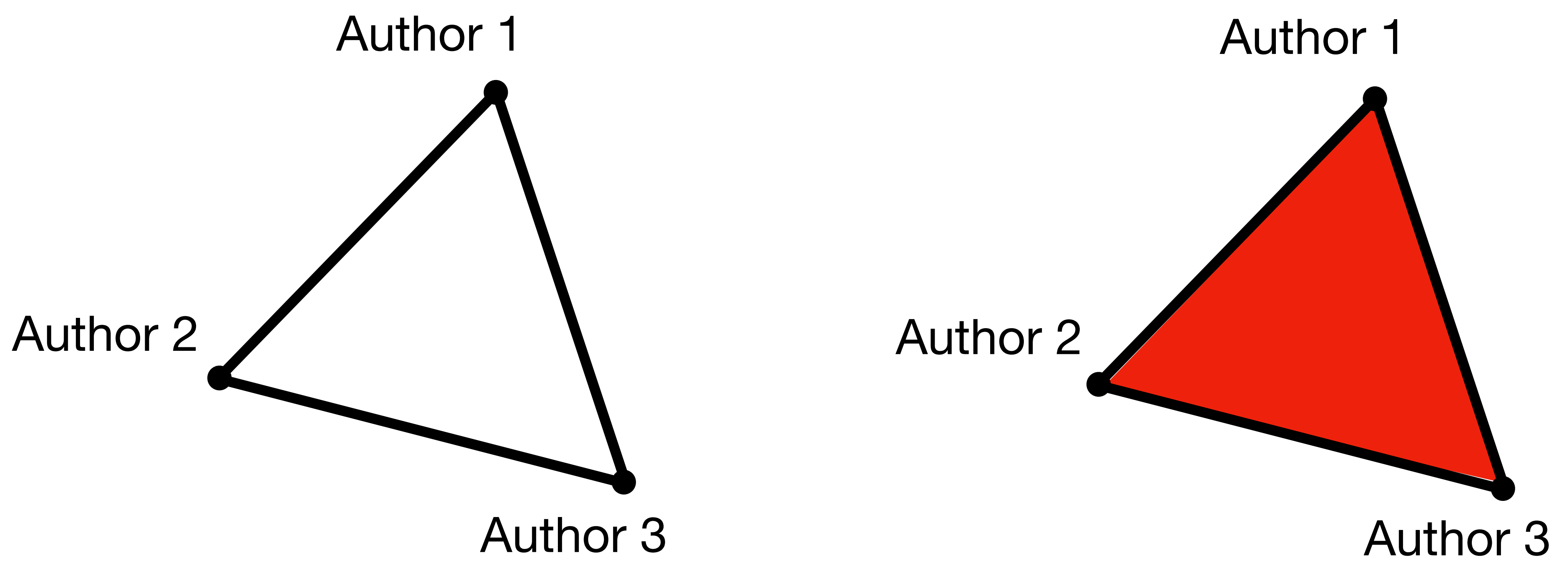
# Higher-order complex networks

## Collaboration networks

**Social network**




**Collaboration network**

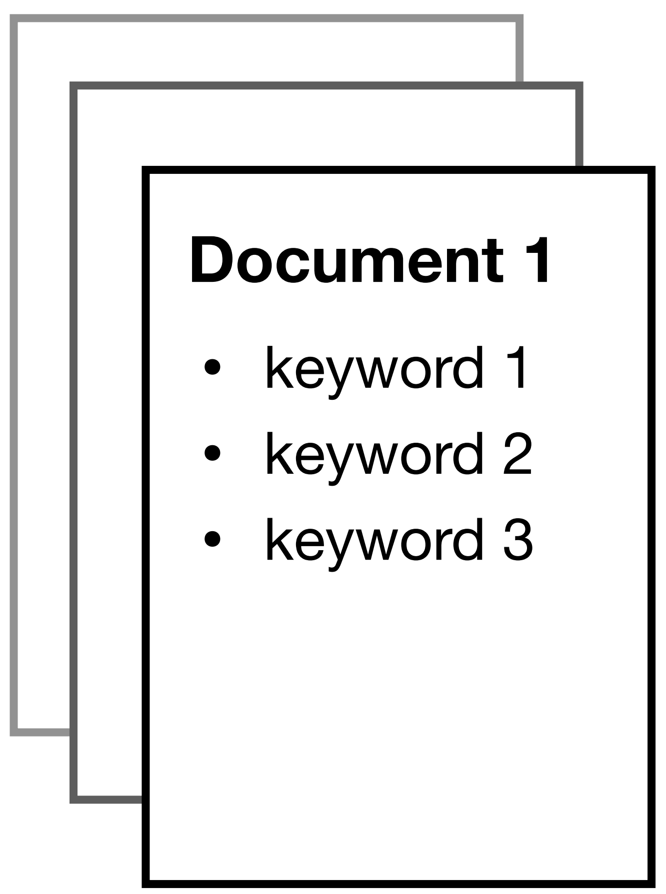



- paper 1 (authors 1-2)
- paper 2 (authors 1-3)
- paper 3 (authors 2-3)

- paper 4 (Authors 1-2-3)

# Higher-order complex networks

## Co-occurence networks




**Word-document matrix**

| | Word 1 | Word 2 | Word 3 |
|---|---|---|---|
| Doc 1 | | 1 | |
| Doc 2 | 1 | 1 | |
| Doc 3 | | | 1 |
| Doc 4 | | 1 | |

**Basket 1**

- item 1, item 2, item 3

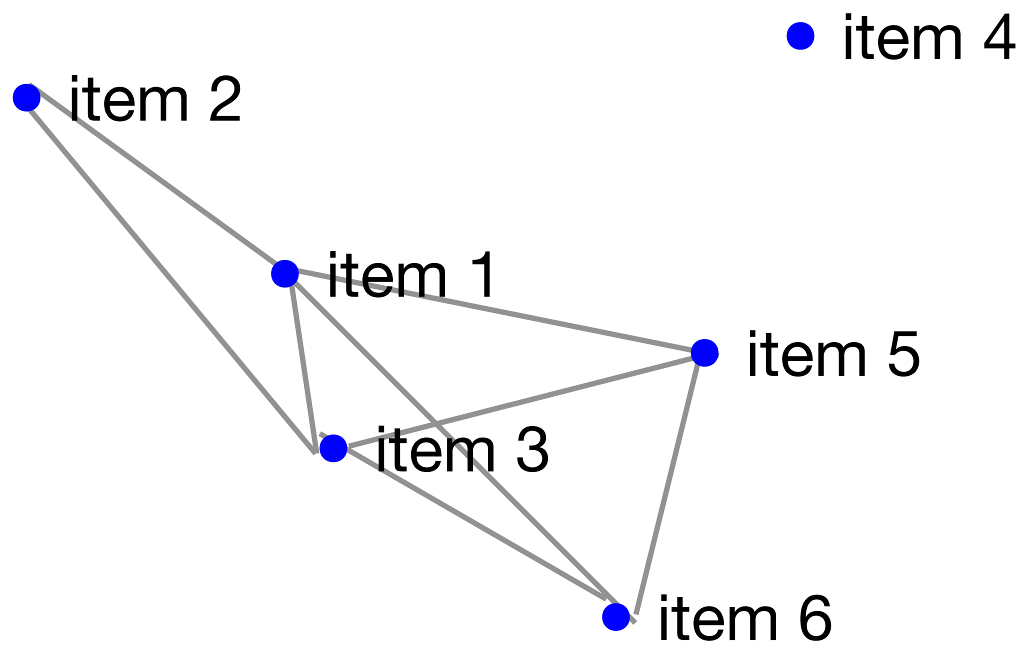
**Basket 2**

- item 1, item 3, item 5, item 6

**Item-basket matrix**

| | Item 1 | … | Item 6 |
|---|---|---|---|
| Basket 1 | 1 | … | |
| Basket 2 | 1 | … | 1 |

**Graph**
Homogenous




**Context 1**

quick brown **fox** jumps over

**Context 2**

brown fox **jumps** over lazy

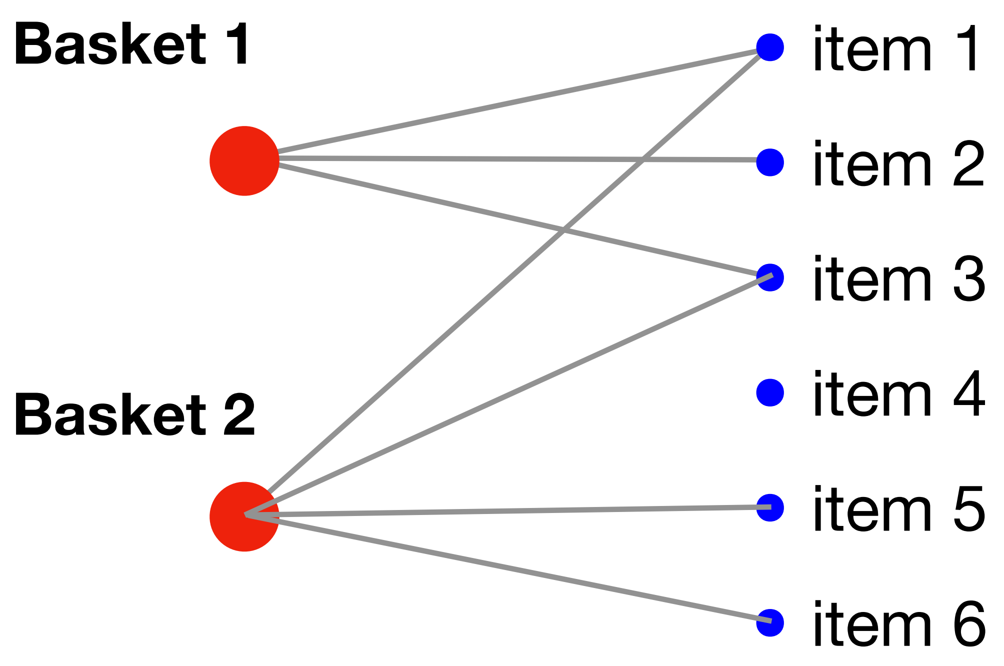
**Context 3**

fox jumps **over** lazy dog

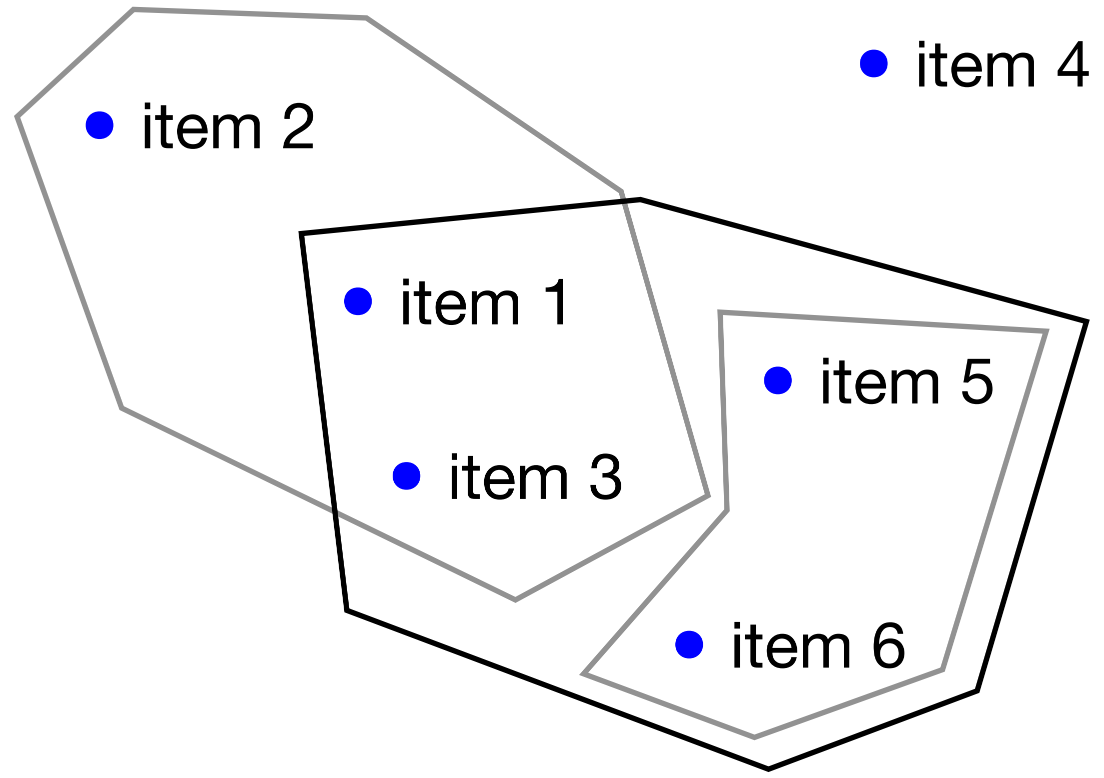
**Word-context matrix**

| | Word 1 | Word 2 | Word 3 |
|---|---|---|---|
| Context 1 | 1 | | |
| Context 2 | 1 | 1 | |
| Context 3 | | 1 | |
| Context 4 | 1 | | 1 |

**Bipartite graph**
Heterogenous

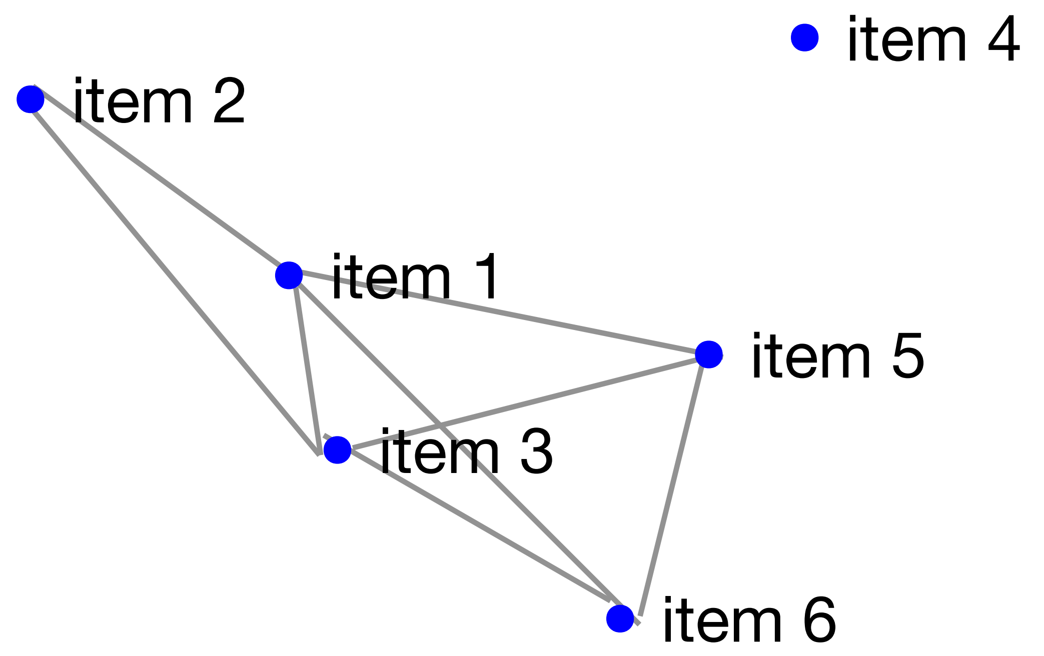



**Hypergraph**
Homogenous

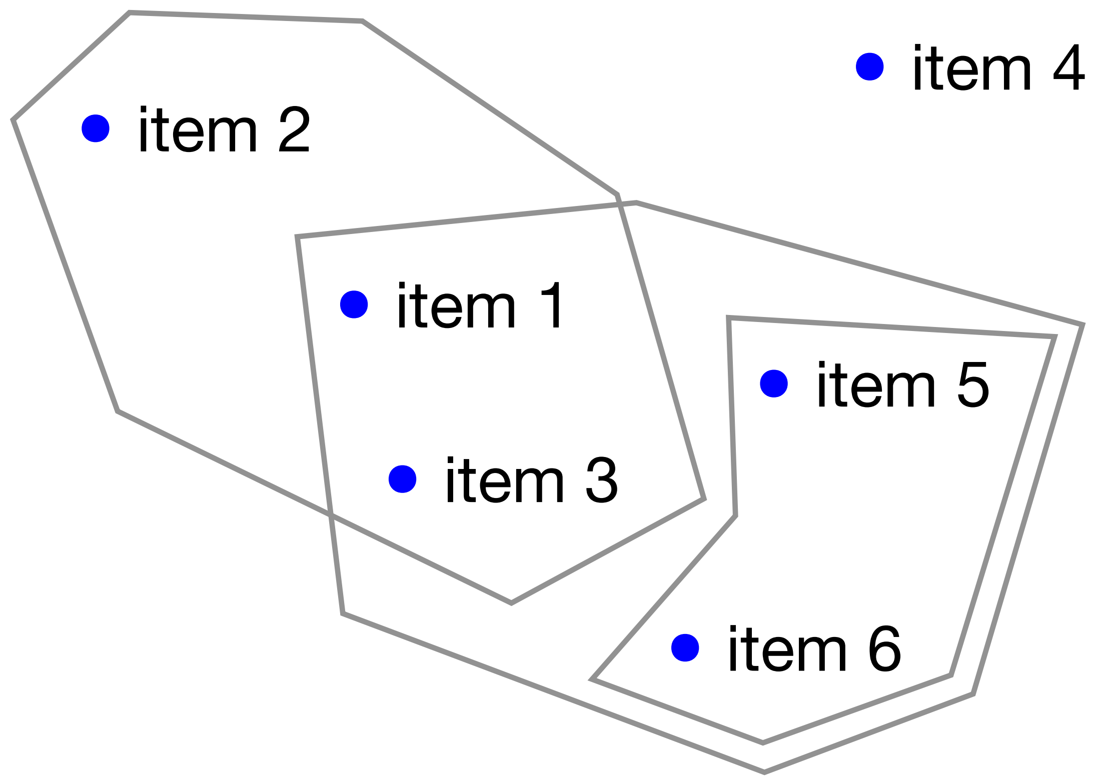


# Higher-order complex networks

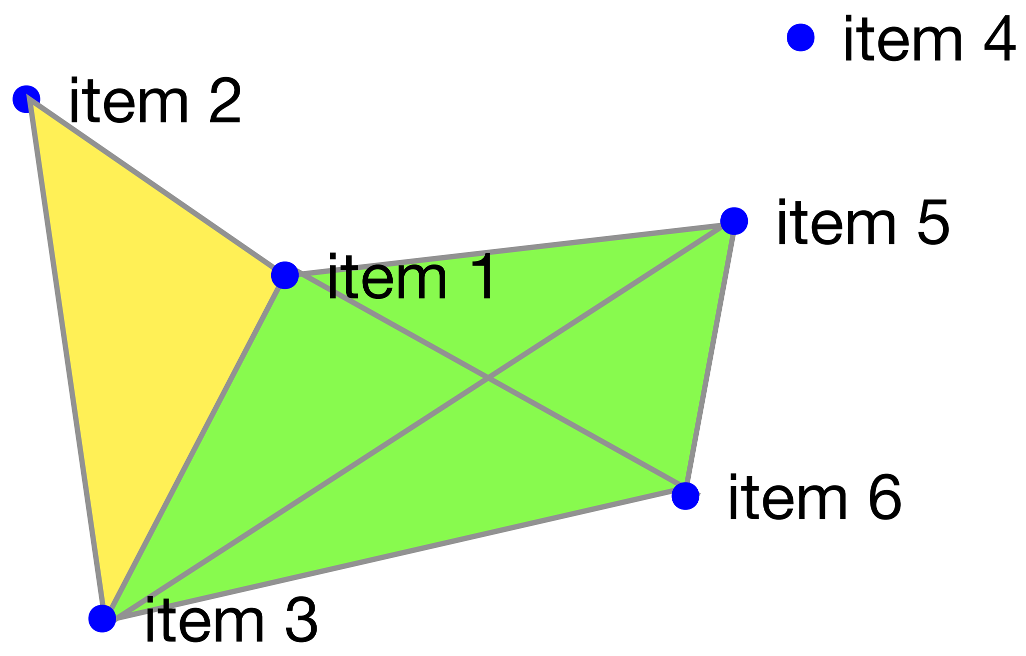
## Models




**Graph**




**Hypergraph**

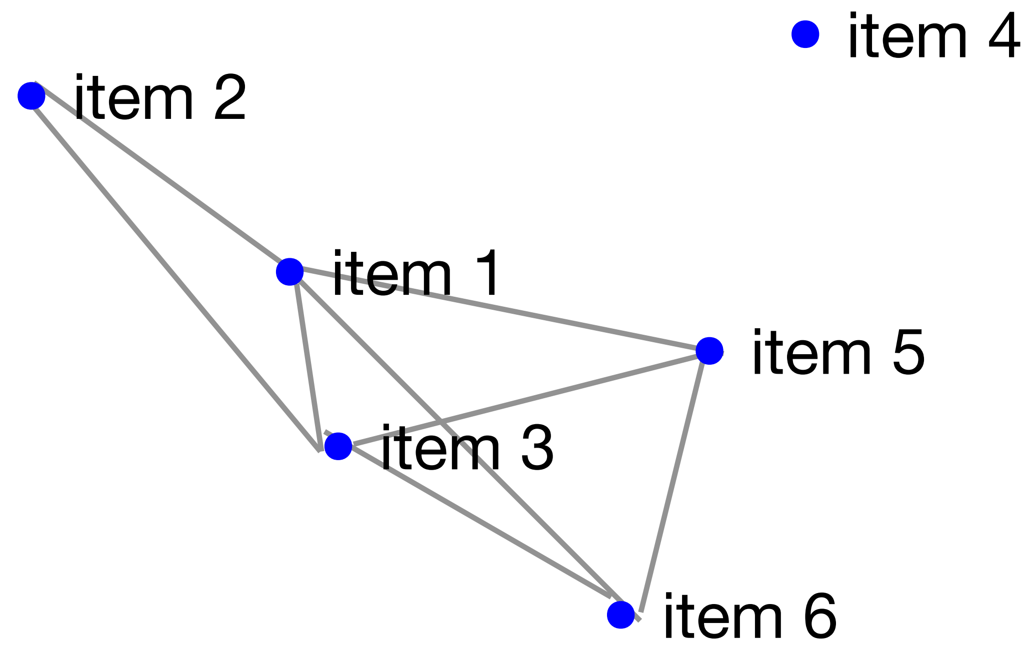



**Simplicial complex**

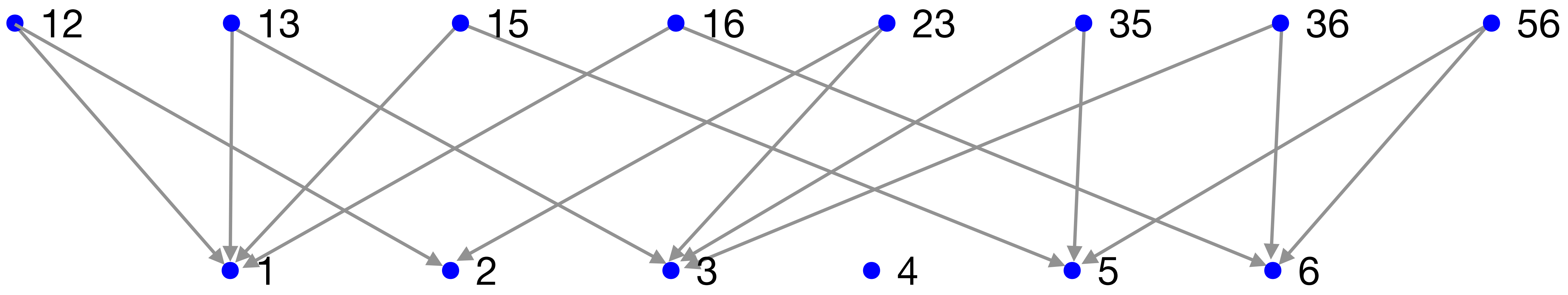
Closed under inclusion
Edges of different dimensions

# Hasse diagram

## Graph



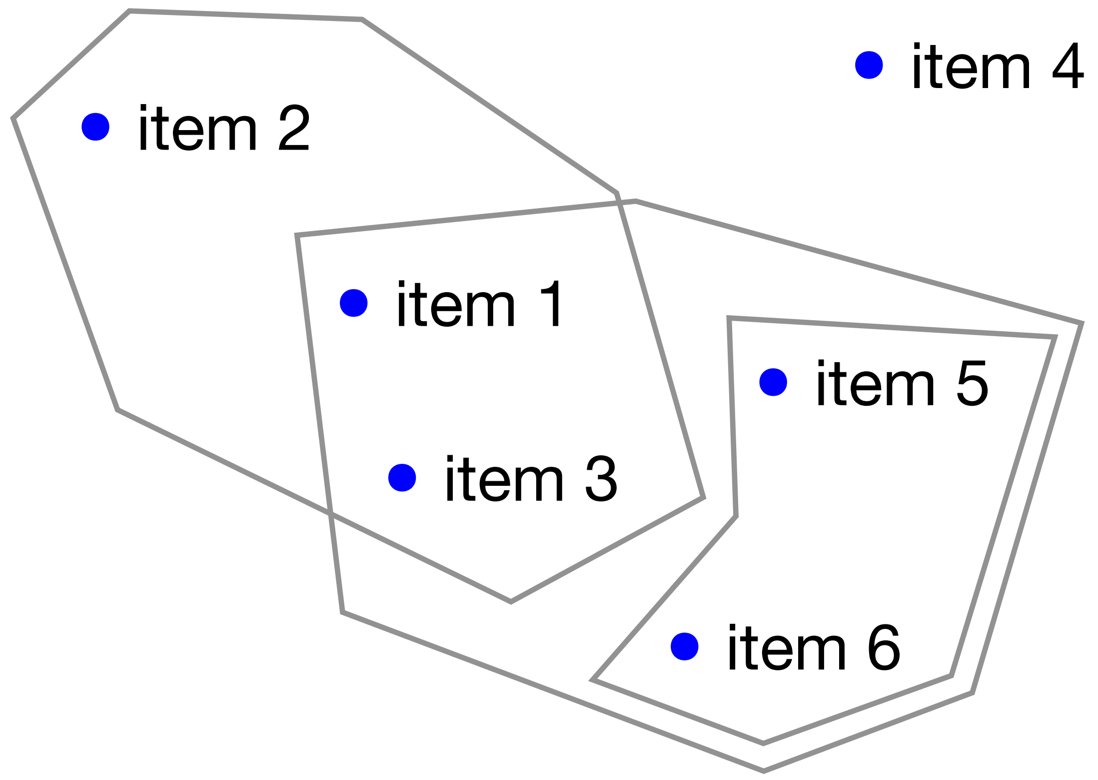

**Graph**



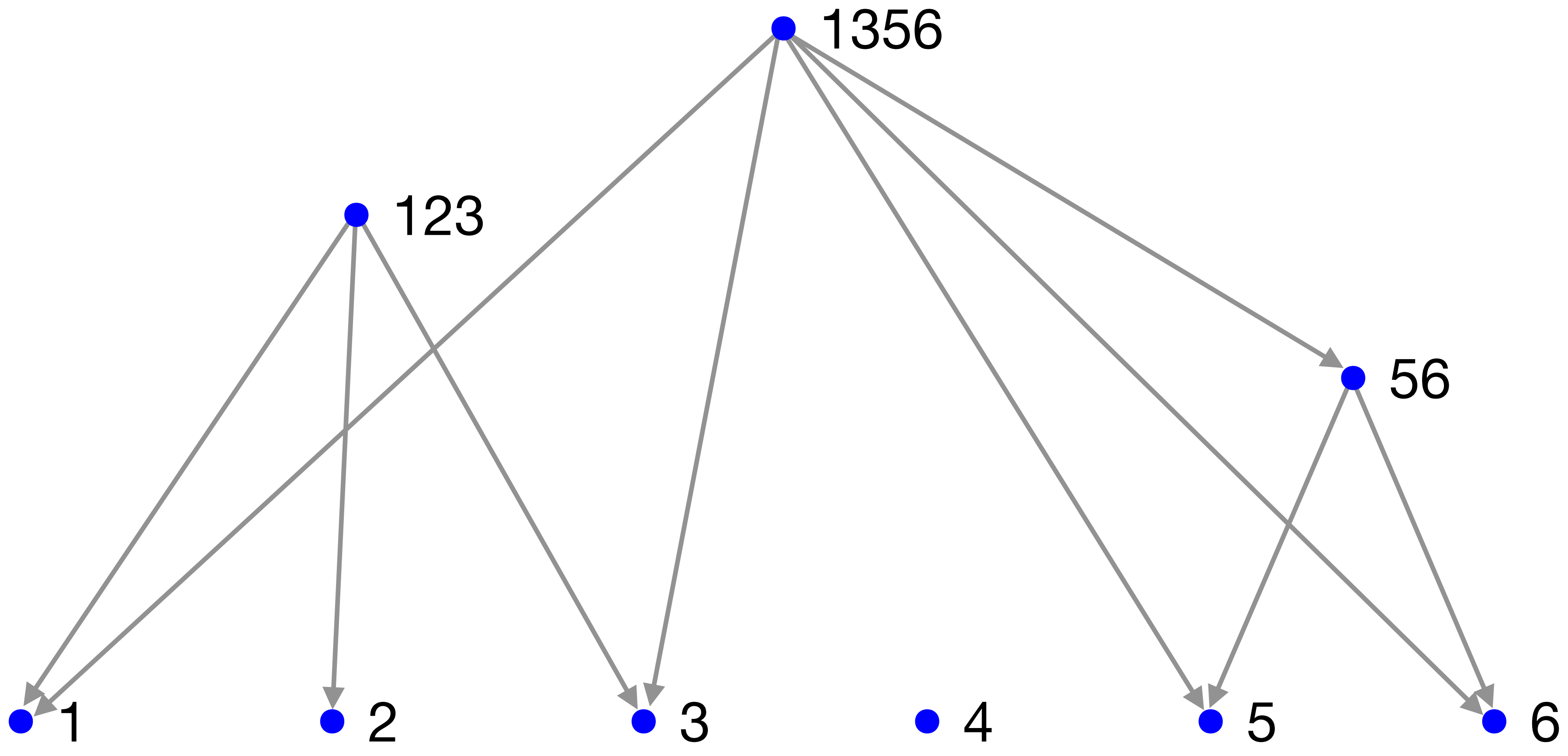

**Hasse diagram**

# Hasse diagram

## Hypergraph



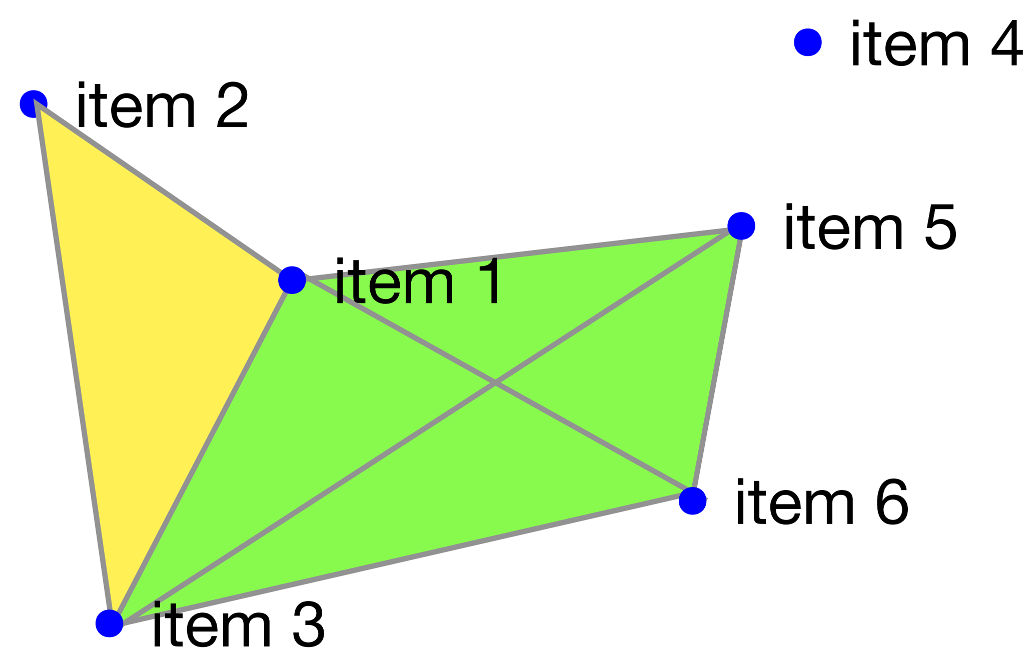

**Hypergraph**



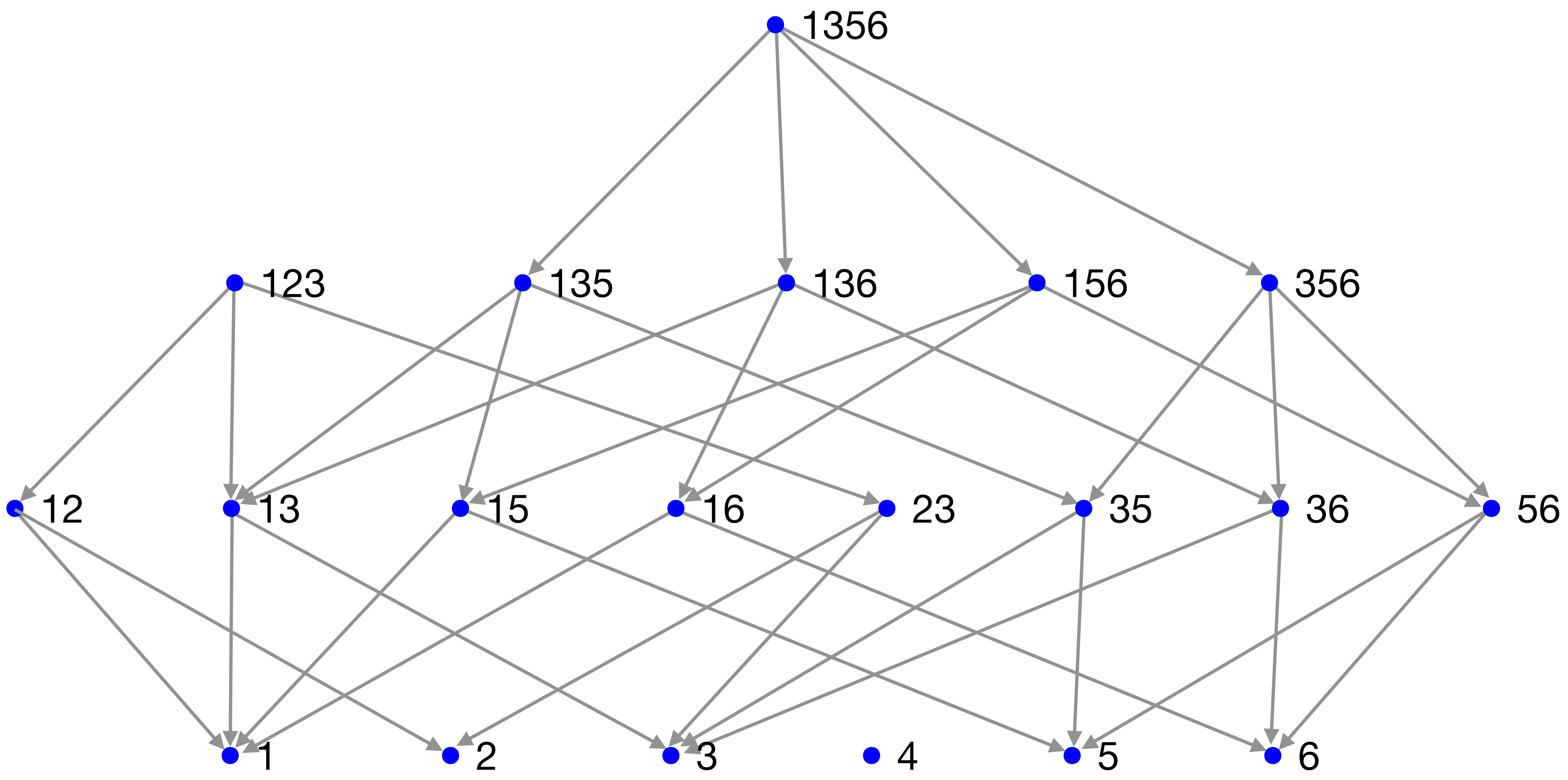

**Hasse diagram**

# Hasse diagram

## Simplicial complex




**Simplicial complex**




**Hasse diagram**

Closed under inclusion
Edges of different dimensions

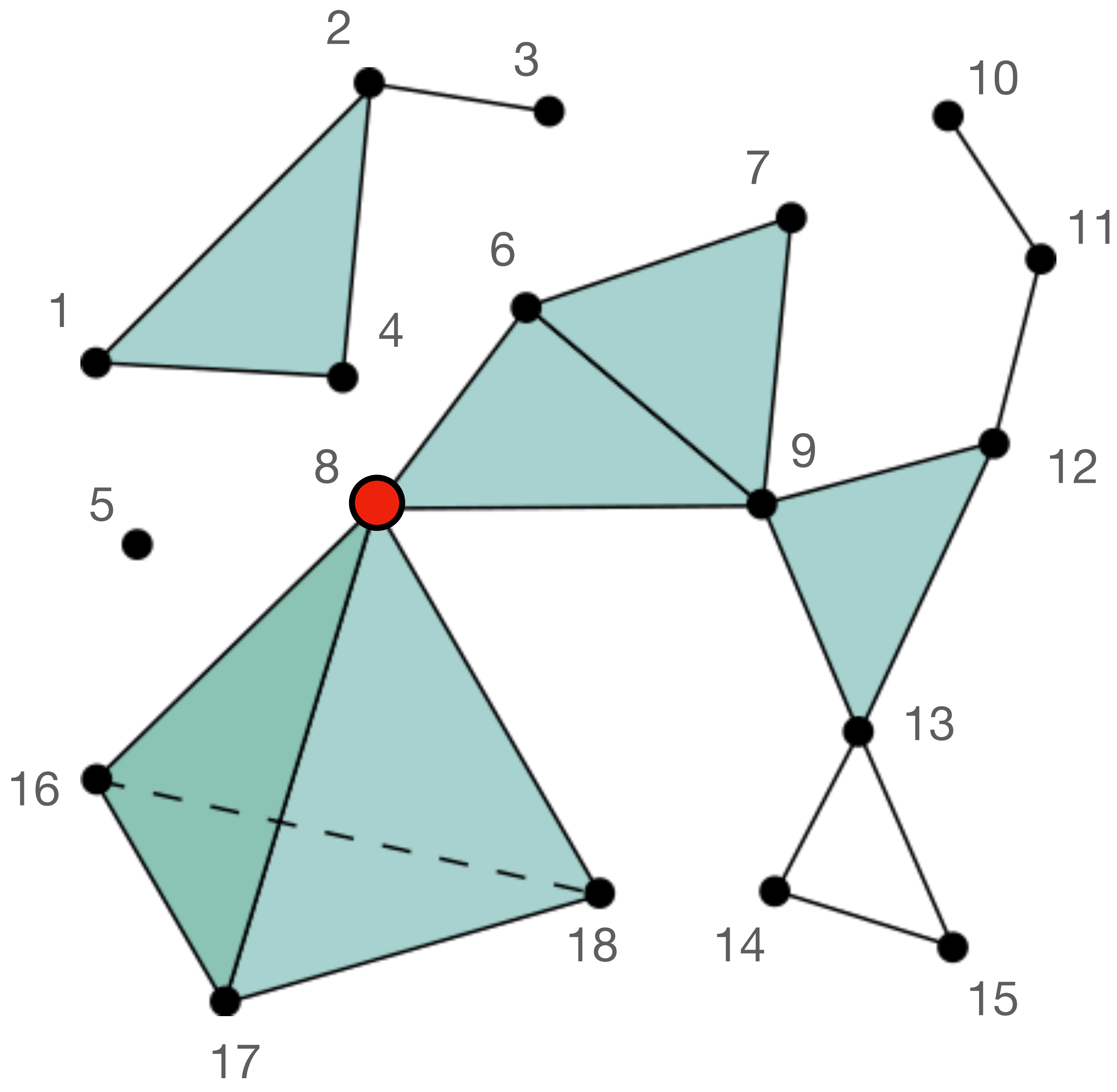
# Incidence, adjacency, degree

## Incidence

For a pair of simplices $\tau \subseteq \sigma$

- $\tau$ is a *face* of $\sigma$,
- $\sigma$ is a *coface* of $\tau$.

A p-simplex $\sigma_1^{(p)}$ is *q-incident* to a q-simplex $\sigma_2^{(q)}$, denoted $\sigma_1^{(p)} \rightarrow_q \sigma_2^{(q)}$ if $p \neq q$ and $\sigma_1^{(p)}$ is a face or coface of $\sigma_2^{(q)}$.




**Simplicial complex *K***

# Incidence, adjacency, degree

## Incidence

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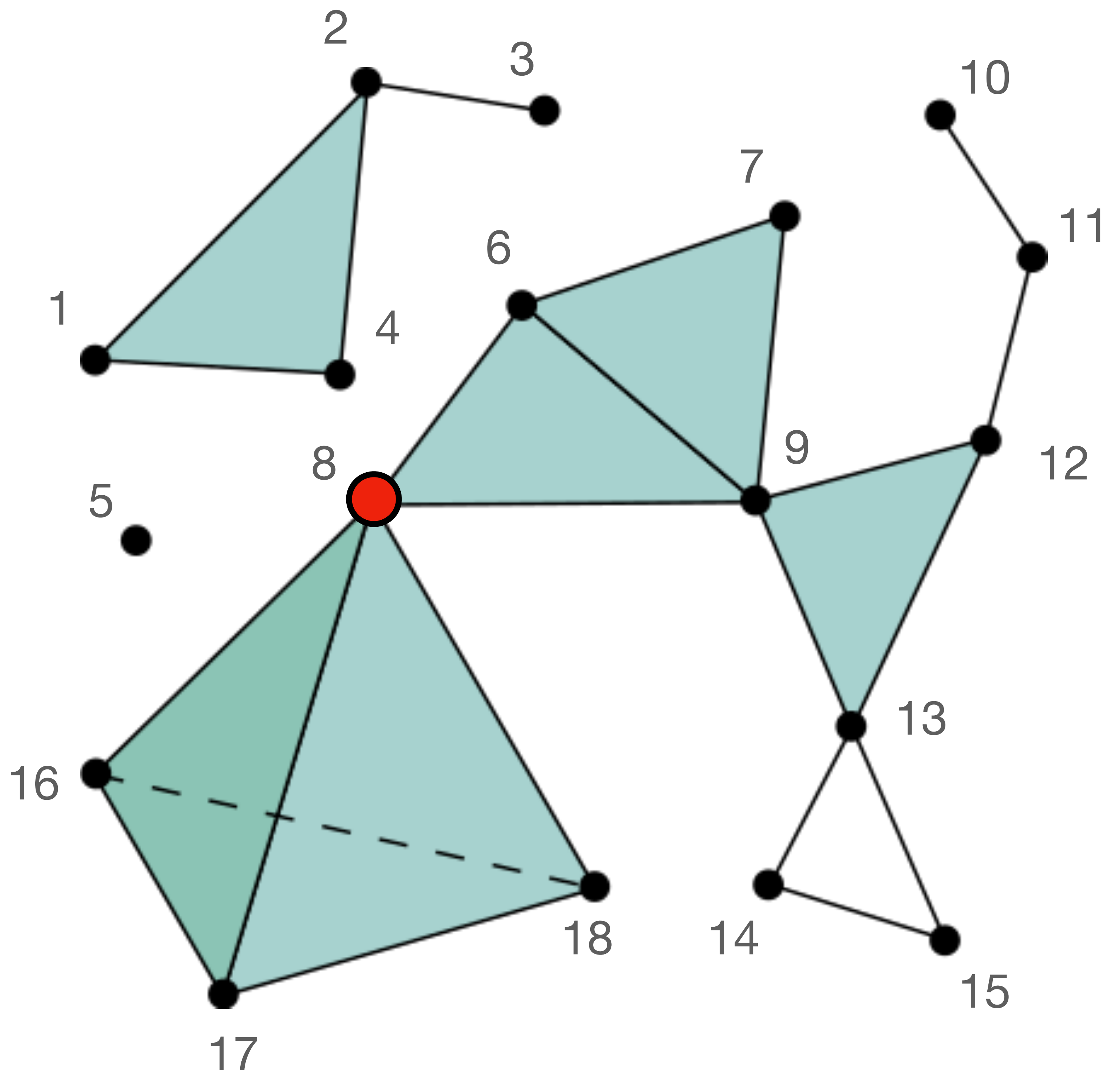
**Upper incidence** $p < q$

$\{8\} \to_1 \{6,8\}$ $\{8\} \to_2 \{8,17,18\}$ $\{8\} \to_3 \{8,16,17,18\}$

$\{8,16\} \to_3 \{8,16,17,18\}$

**Lower incidence** $p < q$

$\{6,7,9\} \to_1 \{6,9\}$ $\{8,16,17,18\} \to_1 \{16,18\}$



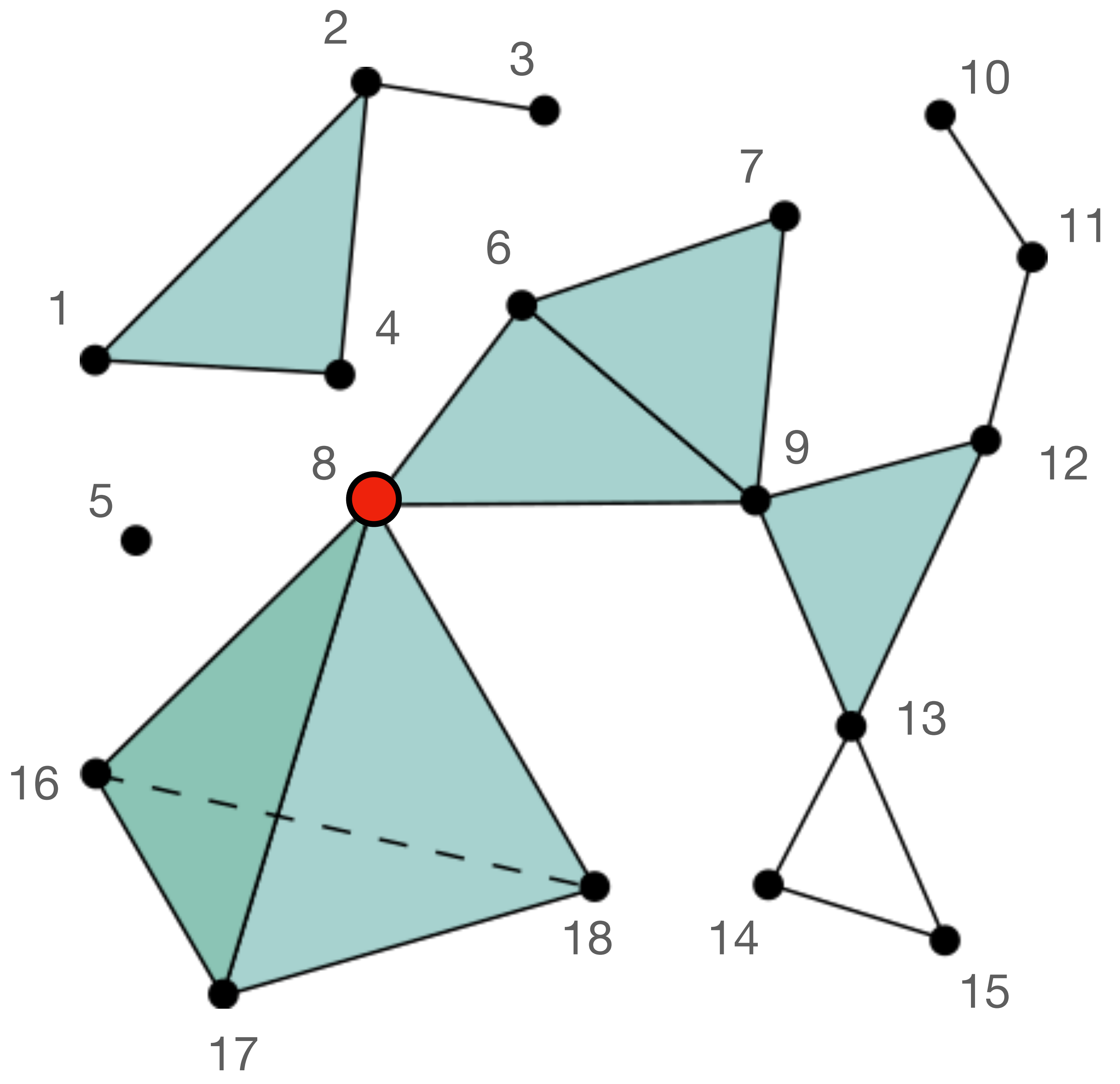

**Simplicial complex *K***

# Incidence, adjacency, degree

## Incidence

*(p, q)-incidence* of a p-simplex is the # q-simplices q-incident to it.

$i_1(\{8\}) = 5$ $\qquad$ $i_2(\{8\}) = 4$ $\qquad$ $i_3(\{8\}) = 1$




**Simplicial complex *K***

# Incidence, adjacency, degree

## Adjacency

A set of p-simplices $\{\sigma_1^{(p)}, \ldots, \sigma_n^{(p)}\}$ is *q-adjacent* via p-simplex $\tau^q$ denoted $\sigma_1^{(p)} \sim_q \sigma_2^{(p)}$ pairwise, or $\sim_q \{\sigma_1^{(p)}, \ldots, \sigma_n^{(p)}\}$ for all p-simplices if

- all p-simplices $\sigma_i^{(p)}$ are p-faces of q-simplex $\tau^{(q)}$, conversely
- q-simplex $\tau^{(q)}$ is a q-coface for all k-simplices $\sigma_i^{(p)}$.

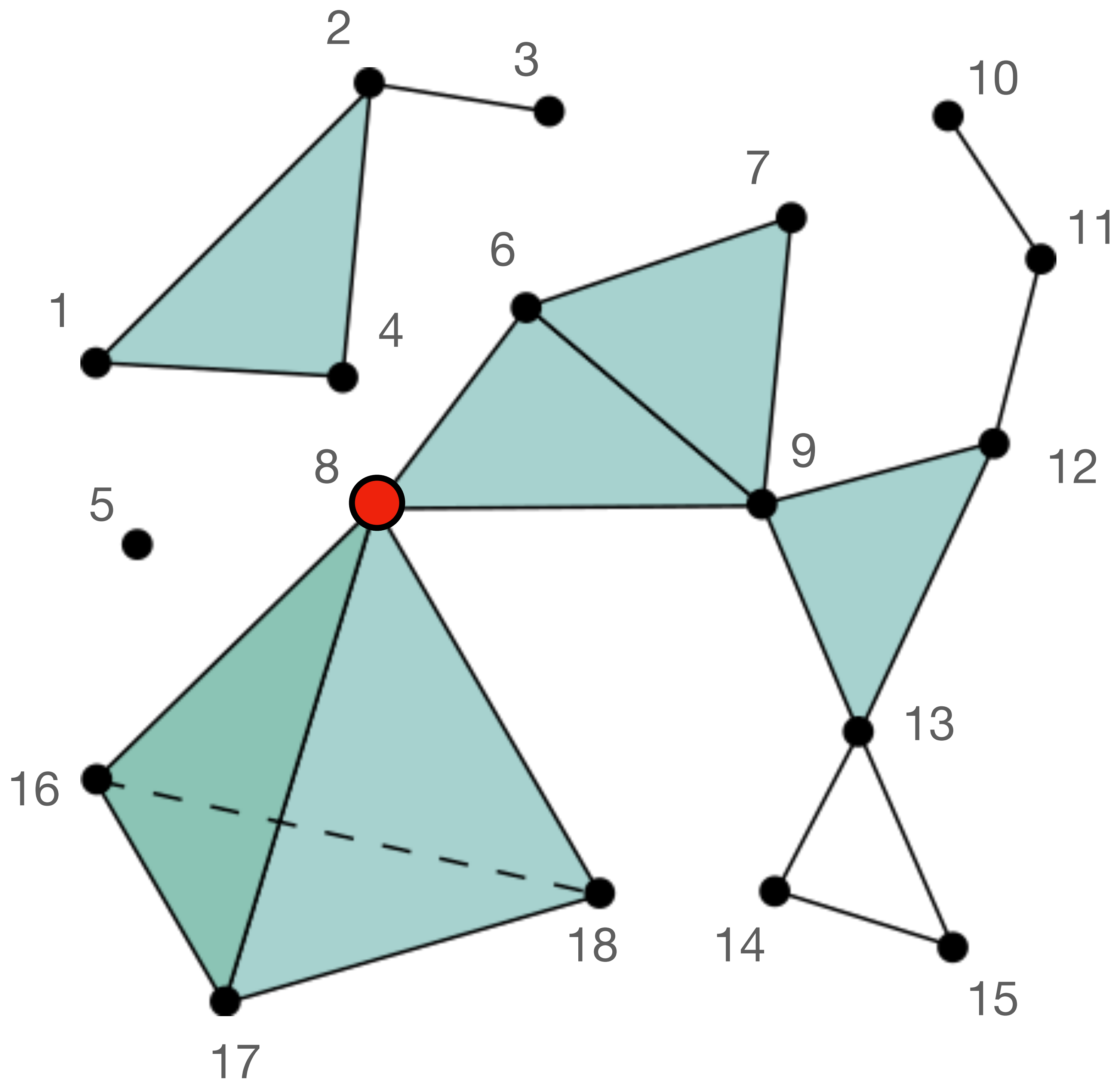
**Upper adjacency** $p < q$

$$\{6{,}9\} \sim_2 \{6{,}7\} \qquad \{8\} \sim_3 \{18\}$$

**Lower adjacency** $p > q$

$$\{8{,}16{,}17\} \sim_0 \{8{,}16{,}17{,}18\} \qquad \{6{,}7{,}9\} \sim_1 \{6{,}8{,}9\}$$

*(p, q)-degree* of a p-simplex is the # of q-adjacent to it p-simplices.



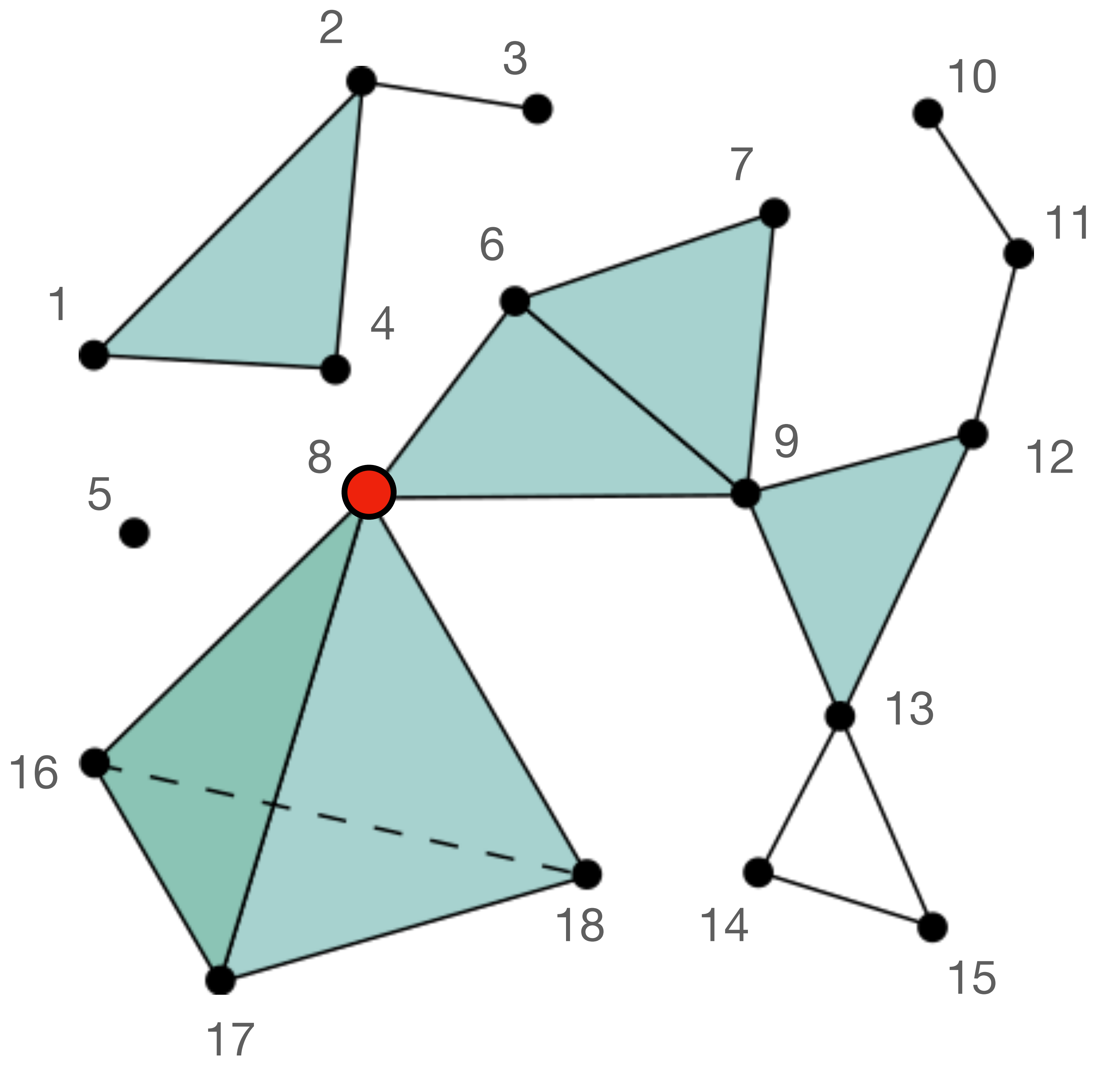

**Simplicial complex *K***

# Incidence, adjacency, degree

## Degree

*(p, q)-degree* of a p-simplex is the # of q-adjacent to it p-simplices.

$$d_1(\{8\}) = 5 \qquad d_2(\{8\}) = 5 \qquad d_3(\{8\}) = 3$$




**Simplicial complex *K***

# Incidence, adjacency, degree

## Degree

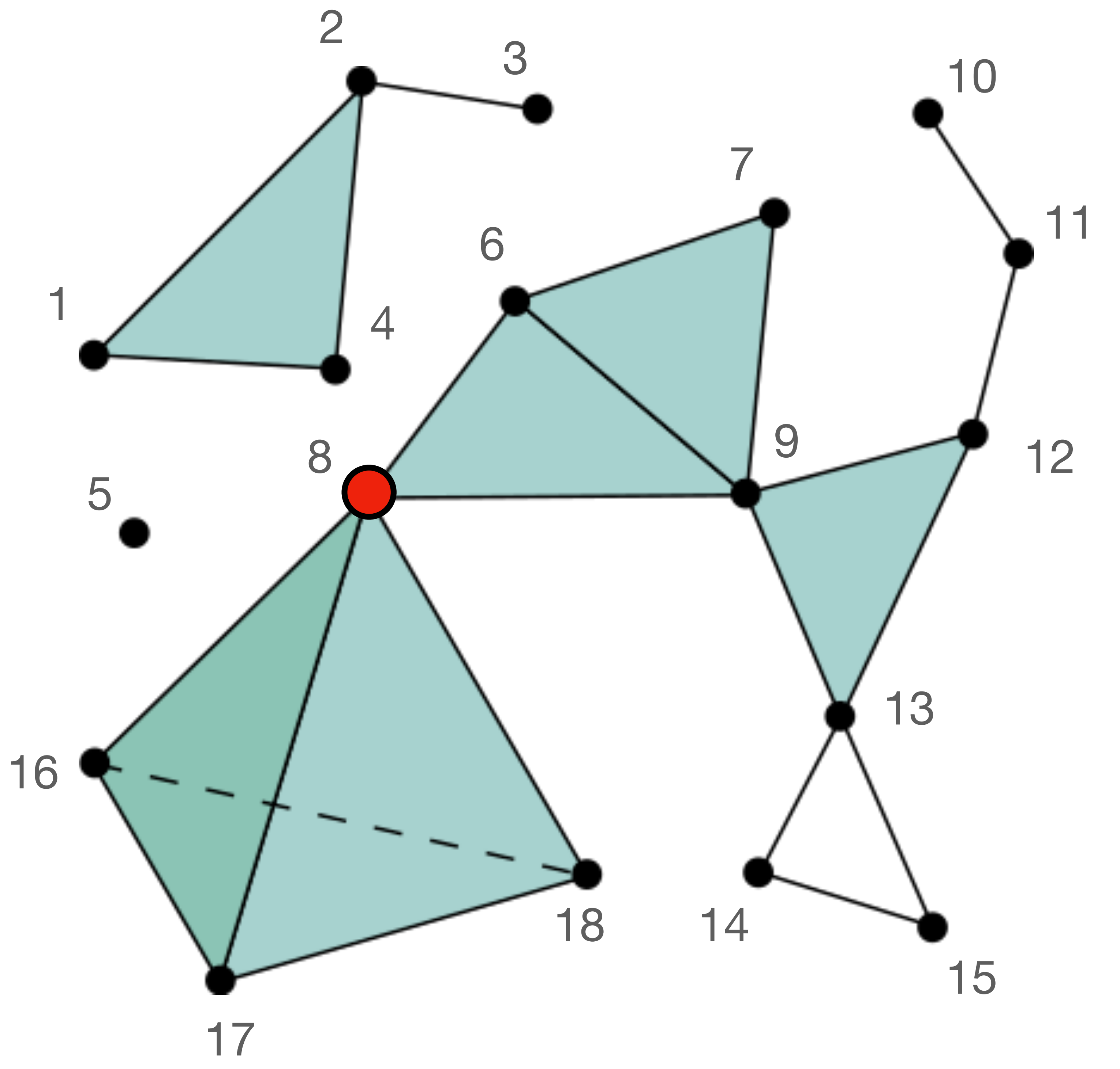
*(p, q)-degree* of a p-simplex is the # of q-adjacent to it p-simplices.

$d_1(\{8\}) = 5$ $\quad d_2(\{8\}) = 5$ $\quad d_3(\{8\}) = 3$

same for q = 1

different for q > 1

$i_1(\{8\}) = 5$ $\quad i_2(\{8\}) = 4$ $\quad i_3(\{8\}) = 1$




**Simplicial complex *K***

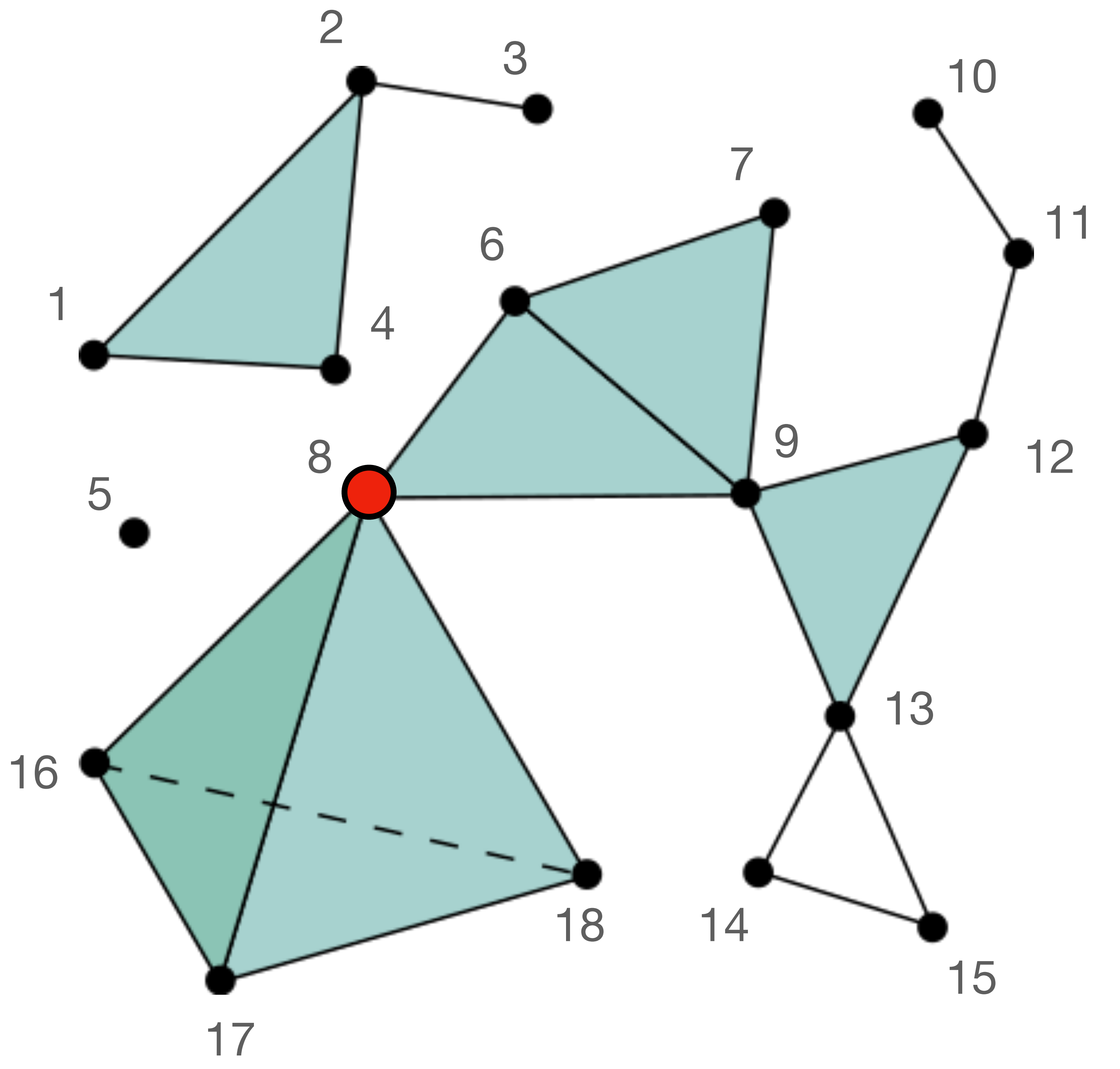
# Connected components

A *(p, q)-path* is a sequence of simplices $\{\sigma_1^{(p)}, \sigma_2^{(q)}, \sigma_3^{(p)}, \sigma_4^{(q)}, \ldots, \sigma_{n-1}^{(q)}, \sigma_n^{(p)}\}$ such that $\sigma_i^{(p)} \rightarrow_q \sigma_{i+1}^{(p)} \rightarrow_q \sigma_{i+2}^{(p)} \quad \forall i$ .

Two simplices $\sigma_1^{(p)}, \sigma_2^{(p)}$ are *(p, q)-connected* if there exists (p, q)-path between them.

A *(p, q)-connected component* is an equivalence relation on *K*.

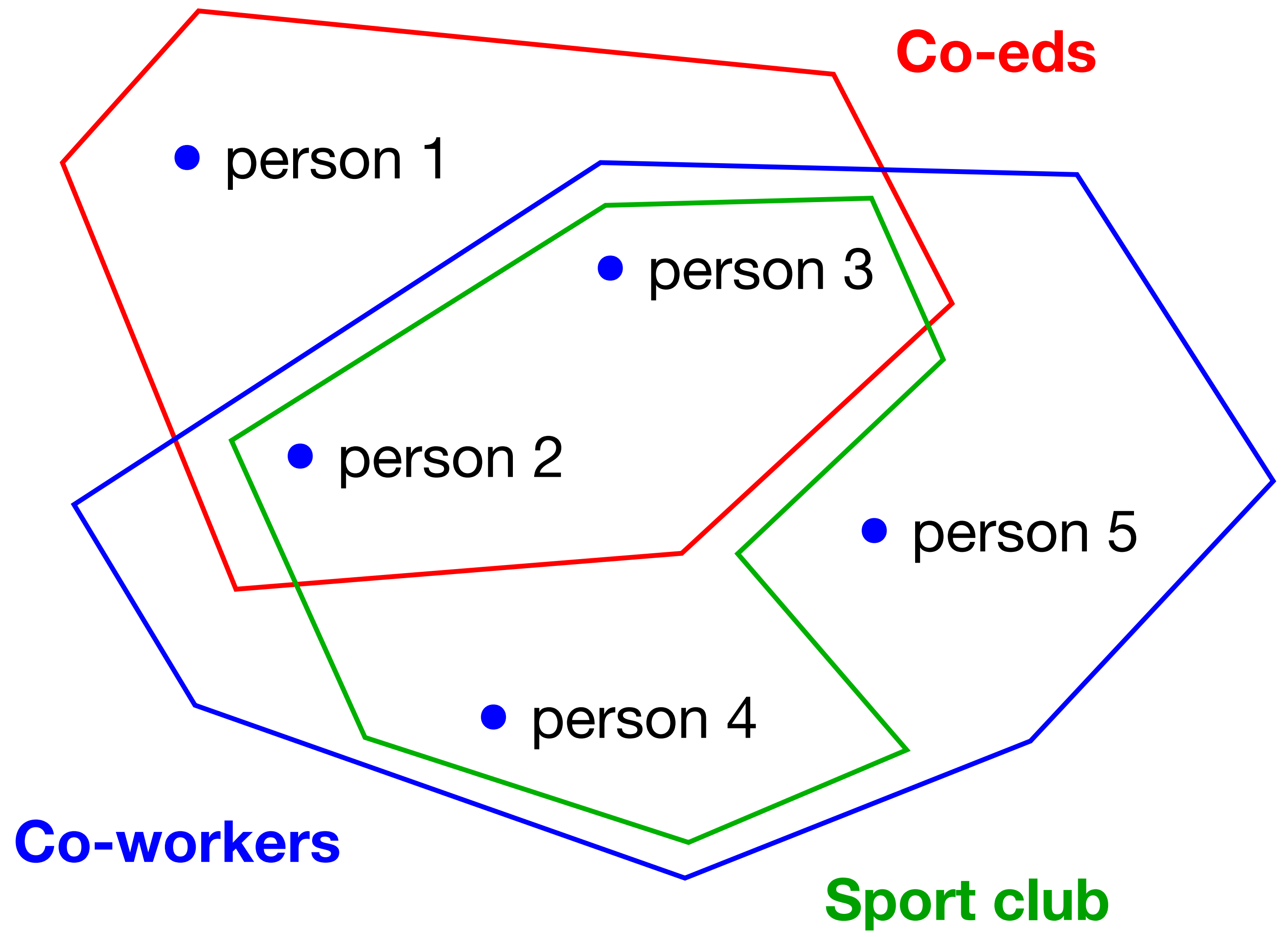
$$|C_{0,1}(K)| = 3 \qquad |C_{0,2}(K)| = 8$$




**Simplicial complex *K***

# Q-analysis

**Social networks**




From Cohomology in Physics to Q-connectivity in Social Science
Atkin R. *International Journal of Man-Machine Studies (1972)*

**Chess networks**

Multi-dimensional Structure in the Game of Chess
Atkin R. *International Journal of Man-Machine Studies (1972)*

# Dowker complex

## Binary relation

Let *X* and *Y* be sets or cardinalities *m* and *n*, respectively

$$X = \{x_1, \ldots, x_m\} \qquad Y = \{y_1, \ldots, y_n\}$$

Binary relation *R* is a subset of Cartesian product *X x Y*

$$R \subseteq X \times Y$$

$$xRy \iff (x, y) \in R$$

**Matrix representation**

*R* on sets *X* and *Y* is represented by m x n matrix ***A***

$$a_{ij} = \begin{cases} 1, & x_i R y_j, \\ 0, & \text{otherwise}. \end{cases}$$

| | $y_1$ | $y_2$ | $y_3$ |
|---|---|---|---|
| $x_1$ | 1 | | |
| $x_2$ | 1 | 1 | |
| $x_3$ | 1 | | 1 |
| $x_4$ | | 1 | 1 |

# Dowker complex

Let R is a binary relation on sets *X* and *Y* of cardinalities *m* and *n*, respectively.

A *Dowker complex K* of a binary relation R on sets X and Y is defined

$$K = \{\sigma^{(m)} = \{x_{\sigma_0}, \ldots, x_{\sigma_m}\} \mid \exists y \text{ s.t. } x_i R y \quad \forall x_i \in \sigma^{(m)}\}$$

Analogously, a *Dowker complex L* is defined

$$L = \{\sigma^{(n)} = \{y_{\sigma_0}, \ldots, y_{\sigma_n}\} \mid \exists x \text{ s.t. } x_i R y \quad \forall y_j \in \sigma^{(n)}\}$$

Homology Groups of Relations
Dowker C. *The Annals of Mathematics (1952)*

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| | $y_1$ | $y_2$ | $y_3$ |
|---|---|---|---|
| $x_1$ | 1 | | |
| $x_2$ | 1 | 1 | |
| $x_3$ | 1 | | 1 |
| $x_4$ | | 1 | 1 |

$\sigma^{(2)} = \{x_1, x_2, x_3\} \in K$

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Analogously, a *Dowker complex L* is defined

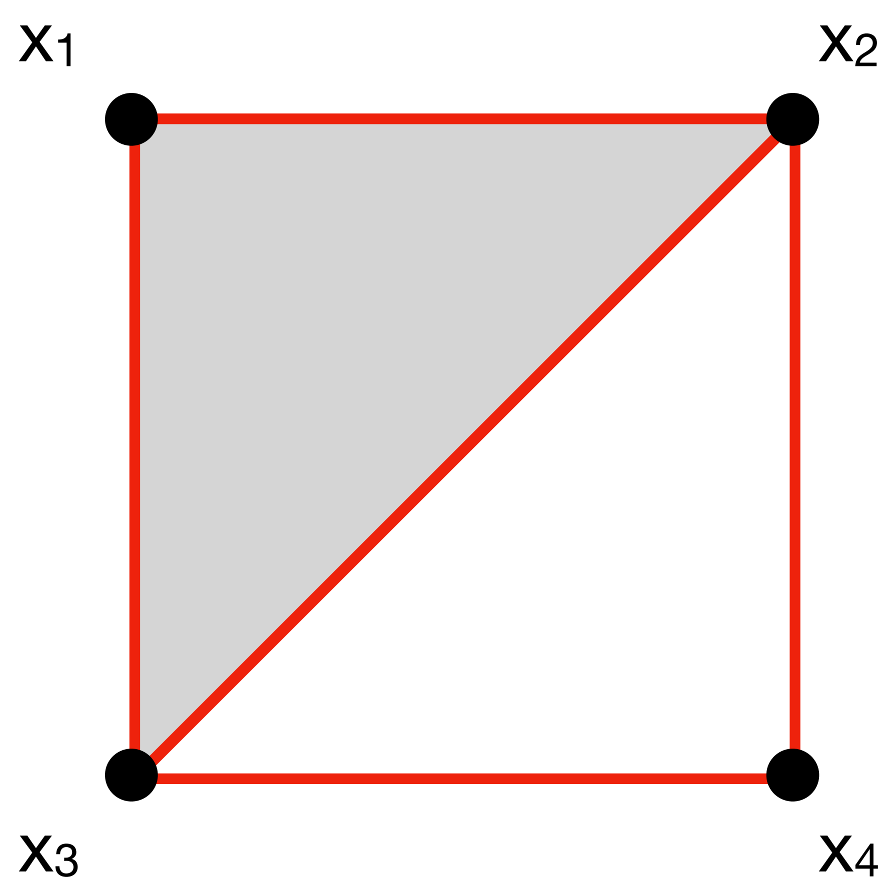
$$L = \{\sigma^{(n)} = \{y_{\sigma_0}, \ldots, y_{\sigma_n}\} \mid \exists x \text{ s.t. } x_i R y \quad \forall y_j \in \sigma^{(n)}\}$$

| | $y_1$ | $y_2$ | $y_3$ |
|---|---|---|---|
| $x_1$ | 1 | | |
| $x_2$ | 1 | 1 | |
| $x_3$ | 1 | | 1 |
| $x_4$ | | 1 | 1 |

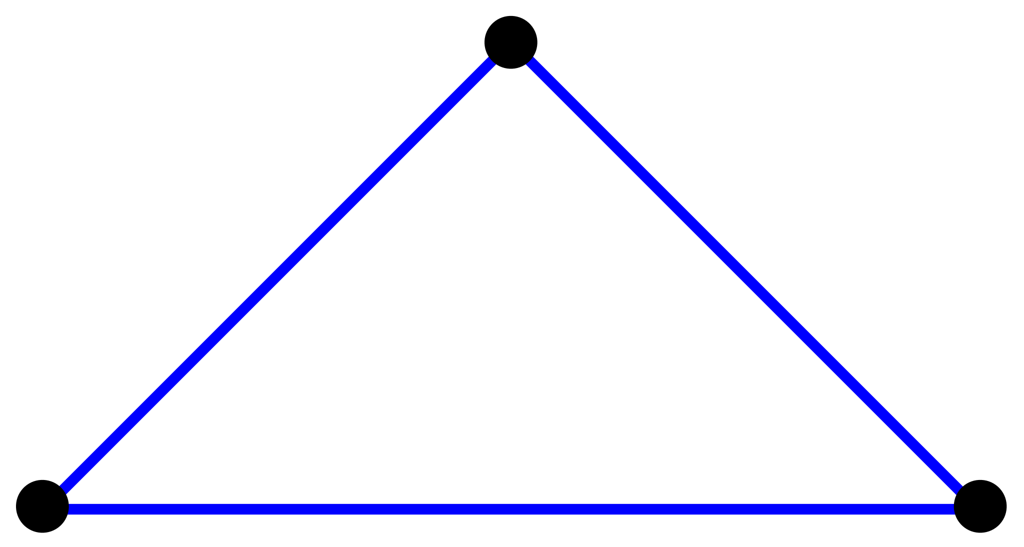
$\sigma^{(1)} = \{y_1, y_3\} \in L$

Homology Groups of Relations
Dowker C. *The Annals of Mathematics (1952)*

# Dowker complex




$K$



$L$

| | $y_1$ | $y_2$ | $y_3$ |
|---|---|---|---|
| $x_1$ | 1 | | |
| $x_2$ | 1 | 1 | |
| $x_3$ | 1 | | 1 |
| $x_4$ | | 1 | 1 |

$\mathbf{A}$

Homology groups of Dowker complexes *K* and *L* are isomorphic, i.e. $H_\bullet(K) \simeq H_\bullet(L)$ [Dowker1952, Thm. 1].

Homology Groups of Relations
Dowker C. *The Annals of Mathematics (1952)*

# Dowker complex

## Chess network

**Chess board**

| | $f_1$ | … | $f_{16}$ |
|---|---|---|---|
| $s_1$ | 1 | | |
| $s_2$ | 1 | 1 | |
| … | 1 | | 1 |
| $s_{64}$ | | 1 | 1 |

**Relation “figure attacks square”**

$K$

**vertices** — figures
**simplices** — squares attacked by a given figure

$L$

**vertices** — squares
**simplices** — figures attacking a given square

**Dowker complexes *K* and *L***

Multi-dimensional Structure in the Game of Chess
Atkin R. *International Journal of Man-Machine Studies (1972)*

# Q-analysis

## Q-connected components

Given a Dowker complex *K (L)* Atkin's Q-analysis is to associate a Q-vector defined as a vector of #(max, q)-connected components of *K (L)* for all *q.*

**Q-vector of *K***

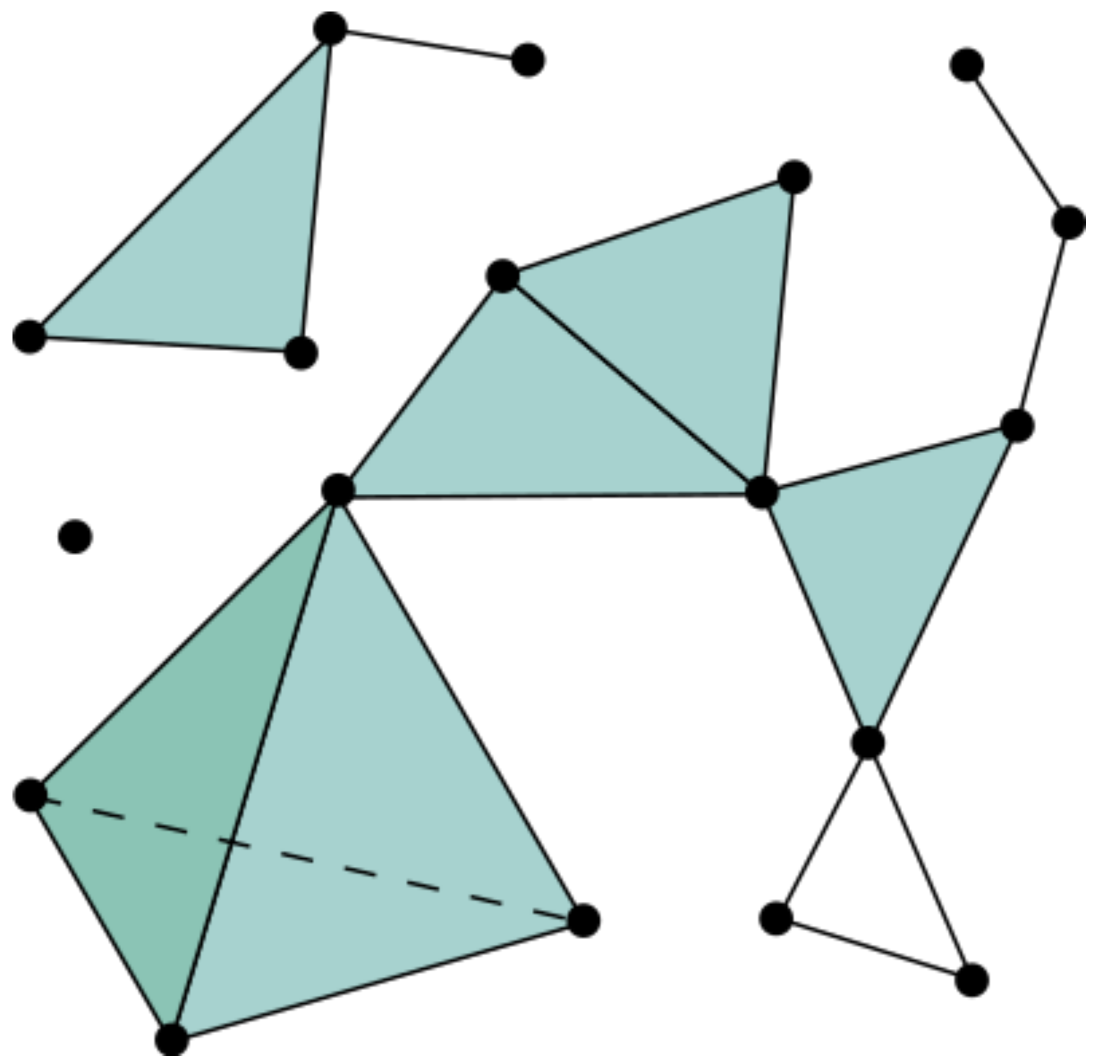
$$(3,\ 4 + m)$$

0 1

**(0, q)-vector of *K***

$$(3,\ 6,\ 15)$$

1 2 3



*K*

**F-vector** $(18,\ 19,\ 8,\ 1)$

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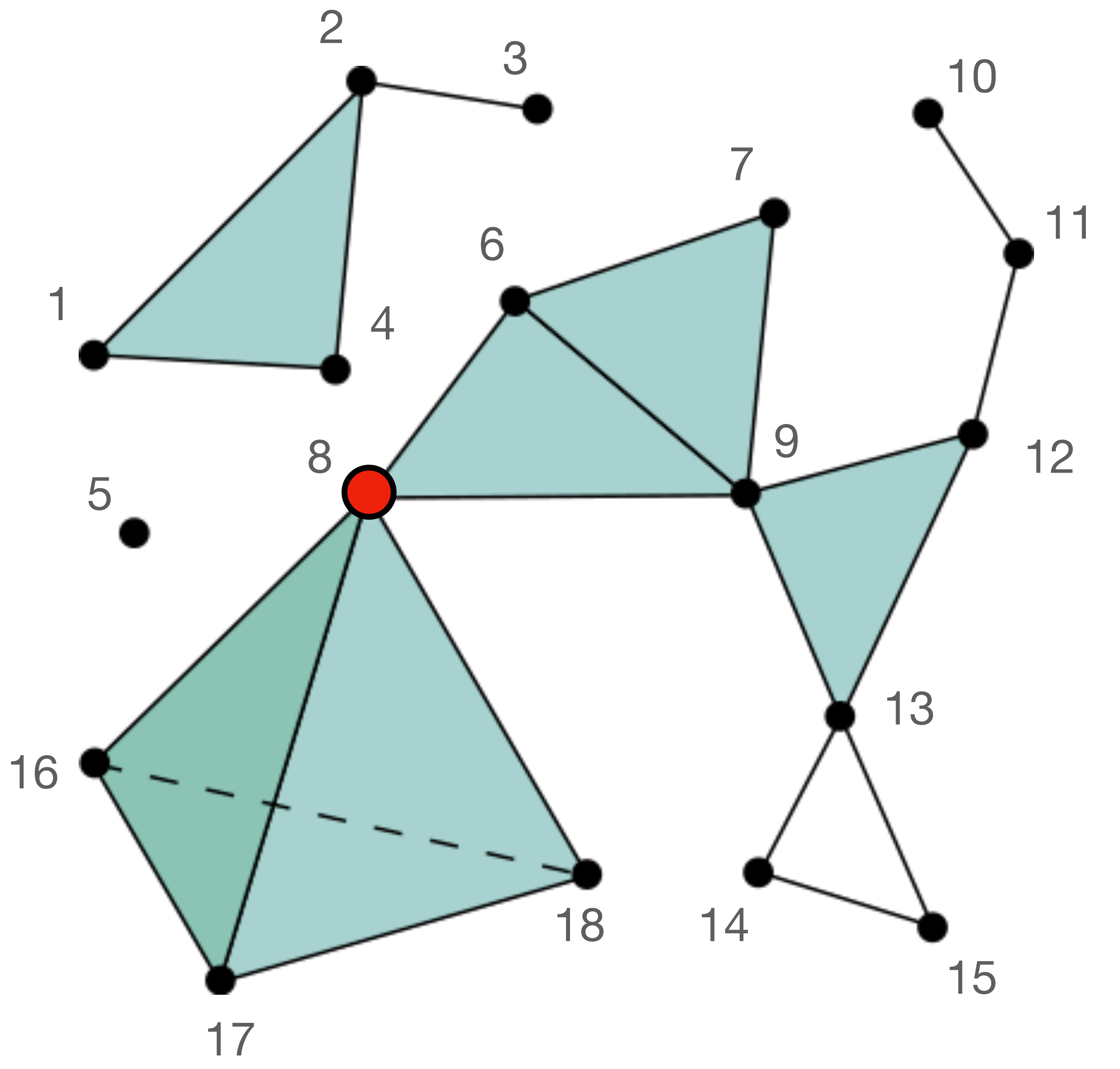
# Line graph

A *(p, q)-line graph* of a simplicial complex *K* is a graph *G(V, E)* where

- *V* consists of p-simplices of *K,*
- $(\sigma_1^{(p)}, \sigma_2^{(p)}) \in E_G$ if $\sigma_1^{(p)} \sim_q \sigma_2^{(p)}$.



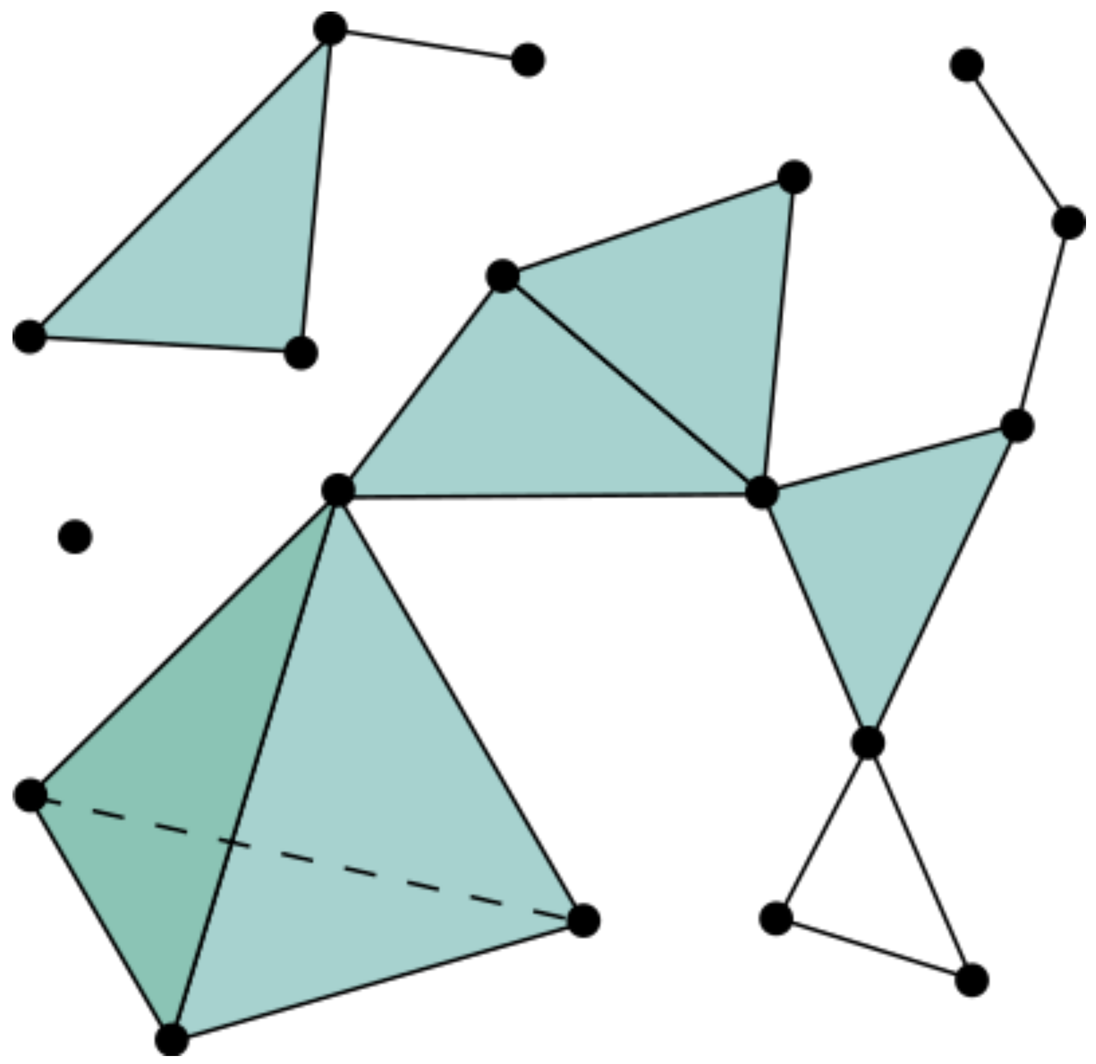

**Simplicial complex *K***

# Centralities

## Betweenness, closeness centrality

**(*p, q*)-betweenness centrality**
# shortest (*p, q*)-paths passing through given *p*-simplex

**(*p, q*)-closeness centrality**
Inverse of sum of the length of (*p, q*)-paths between given *p*-simplex and other *p*-simplices



$K$

Can be computed using (p, q)-line graph

# Higher-order Laplacian

**Chain complex of *K***

$$C_3 \xrightarrow{\partial_3} C_2 \xrightarrow{\partial_2} C_1 \xrightarrow{\partial_1} C_0 \xrightarrow{\partial_0} 0$$

**Higher-order Laplacian operator**

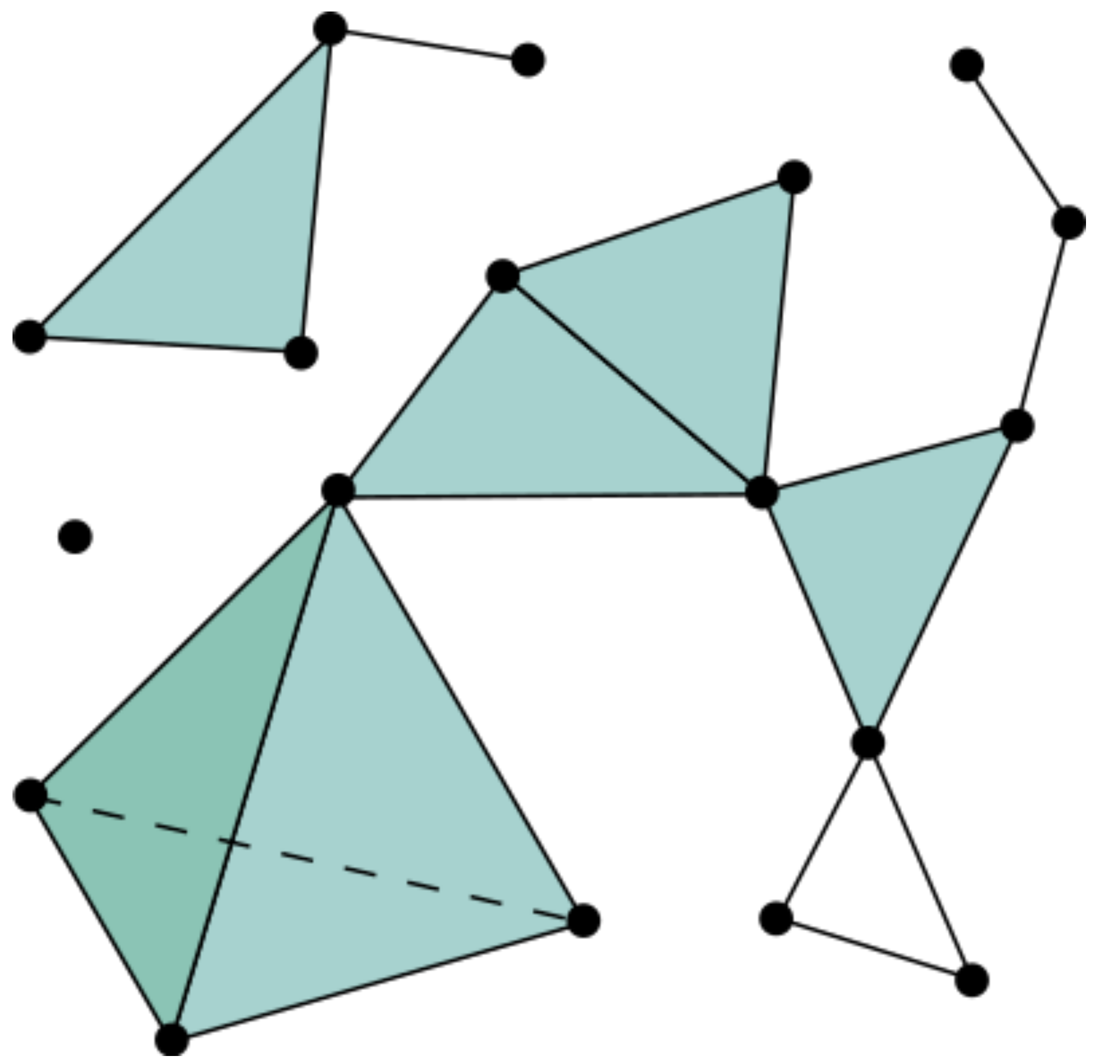
$$C_2 \underset{\partial_2^*}{\overset{\partial_2}{\rightleftarrows}} C_1 \underset{\partial_1^*}{\overset{\partial_1}{\rightleftarrows}} C_0$$

$$\mathbf{L}_p = \mathbf{B}_p^T\mathbf{B}_p + \mathbf{B}_{p+1}\mathbf{B}_{p+1}^T$$

**Graph Laplacian operator**

$$\mathbf{L} = \mathbf{B}\mathbf{B}^T \qquad \mathbf{L} = \mathbf{D} - \mathbf{A}$$

$$\mathbf{L}_0 = \mathbf{B}_1\mathbf{B}_1^T$$



$K$

# Higher-order Laplacian
## Spectrum

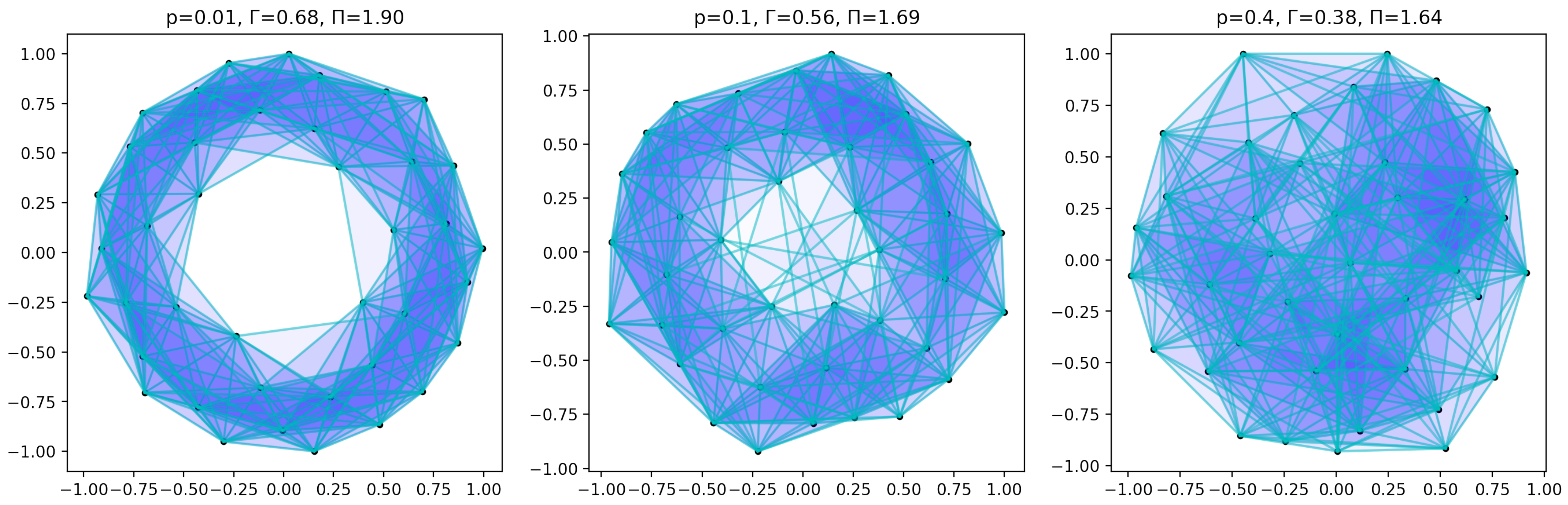
**Higher-order Laplacian operator**

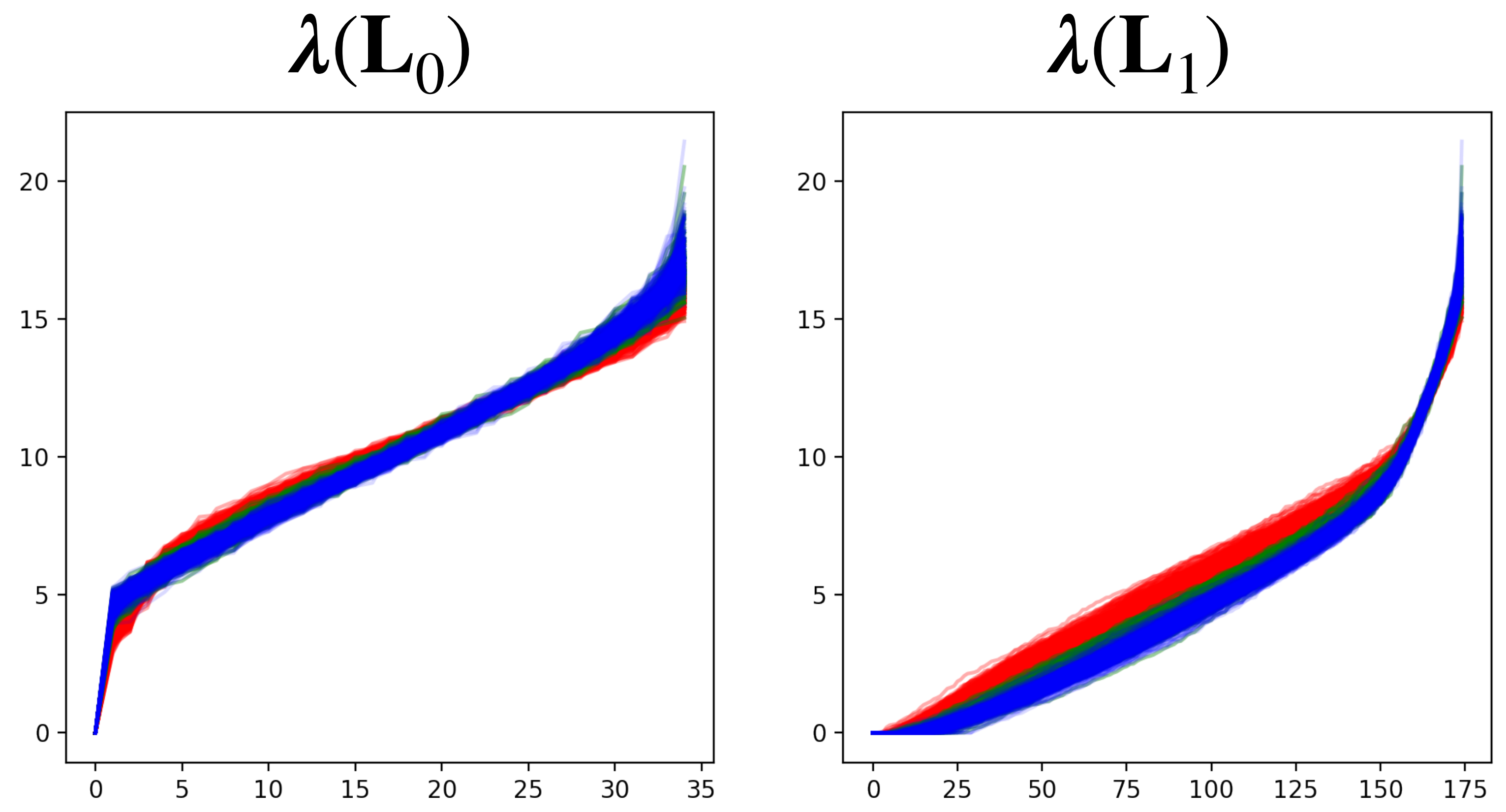
$$C_2 \underset{\partial_2^*}{\overset{\partial_2}{\rightleftarrows}} C_1 \underset{\partial_1^*}{\overset{\partial_1}{\rightleftarrows}} C_0$$

$$\mathbf{L}_p = \mathbf{B}_p^T \mathbf{B}_p + \mathbf{B}_{p+1} \mathbf{B}_{p+1}^T$$

**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 |
|---|---|
| 73.91 ± 0.86 | **78.37 ± 0.62** |

Classification accuracy, % for 5-fold cross-validation averaged over 20 runs.