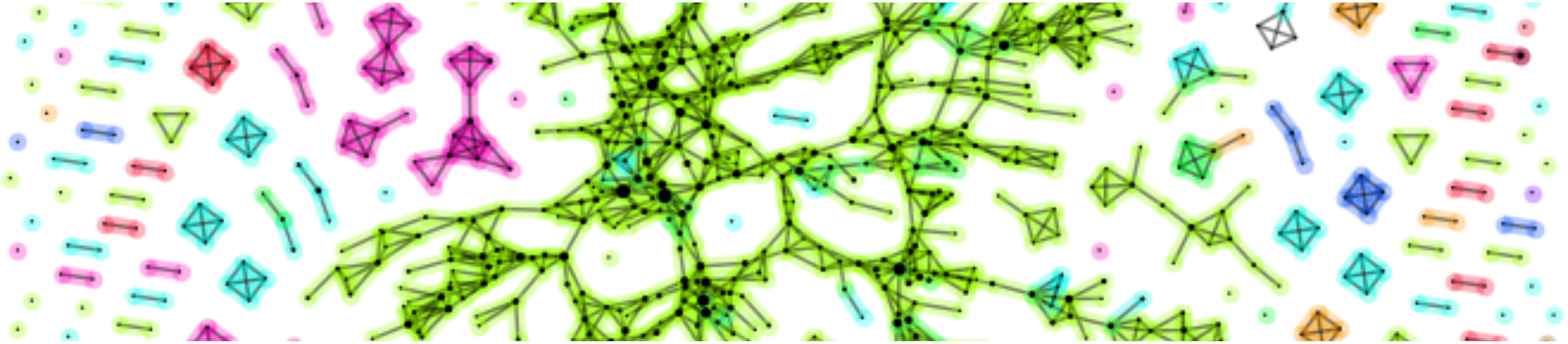
TDA Lecture #1

Introduction, basics and relation to complex systems



G. Petri/P. Expert

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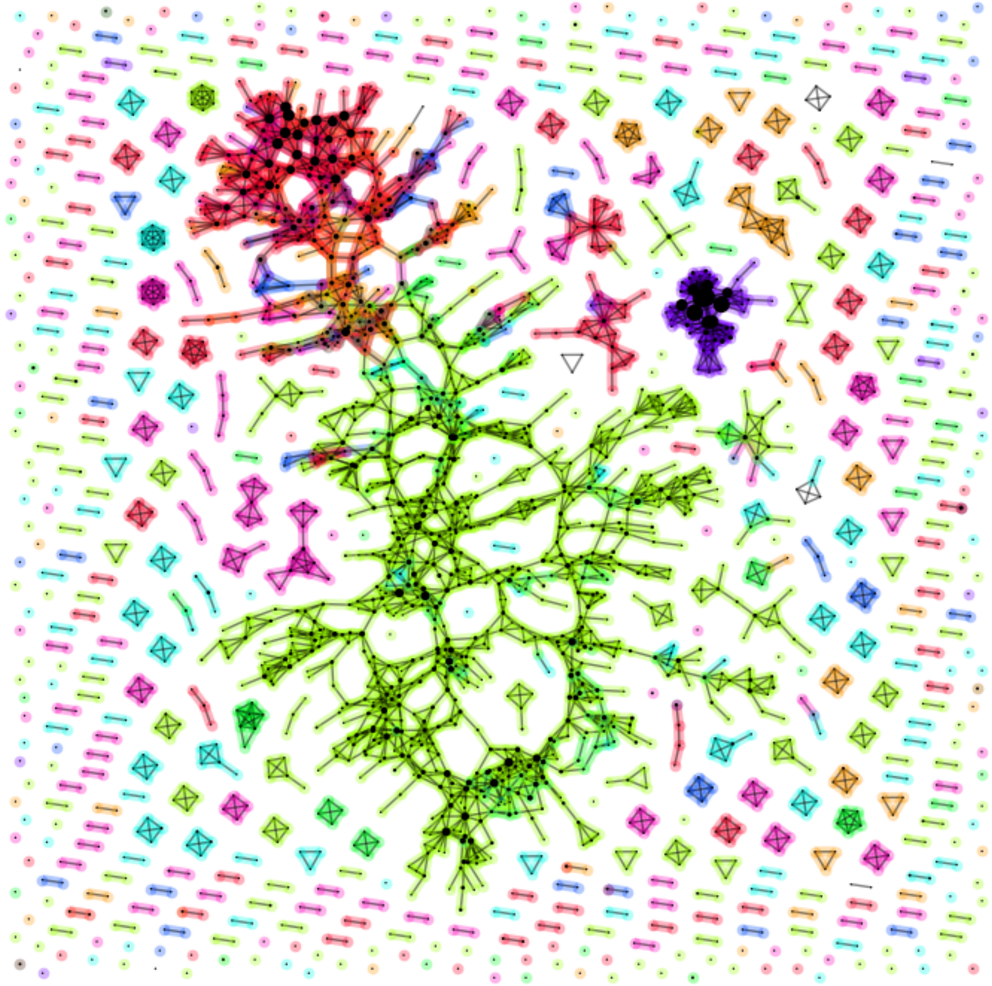
Imperial College
London

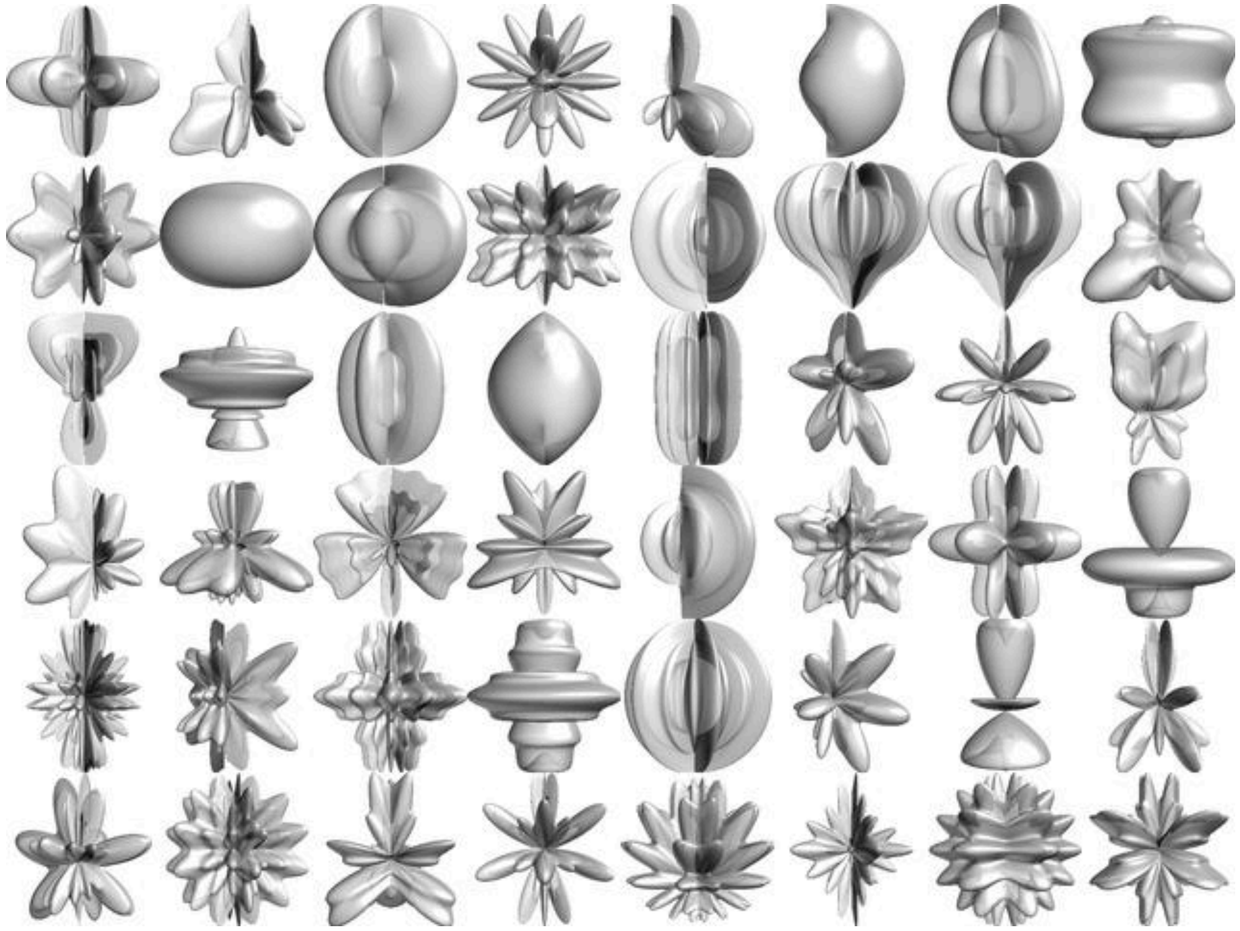
CNTDA2019 , UKM, Kuala Lumpur
Sept 2019

https://github.com/lordgrilo/WCNTDA2019

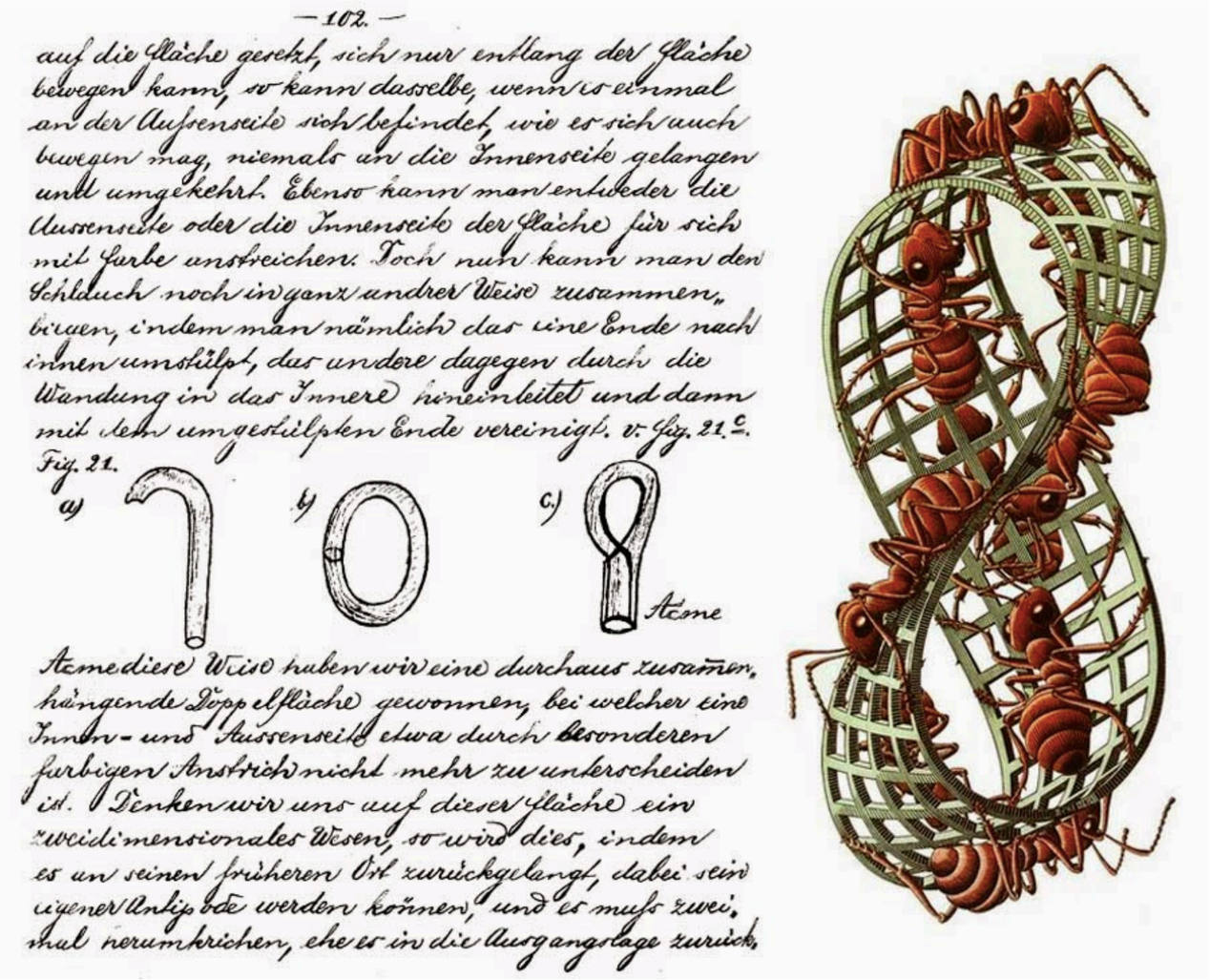
Networks



TDA=shapes



What do we mean by topology?



— 102. —

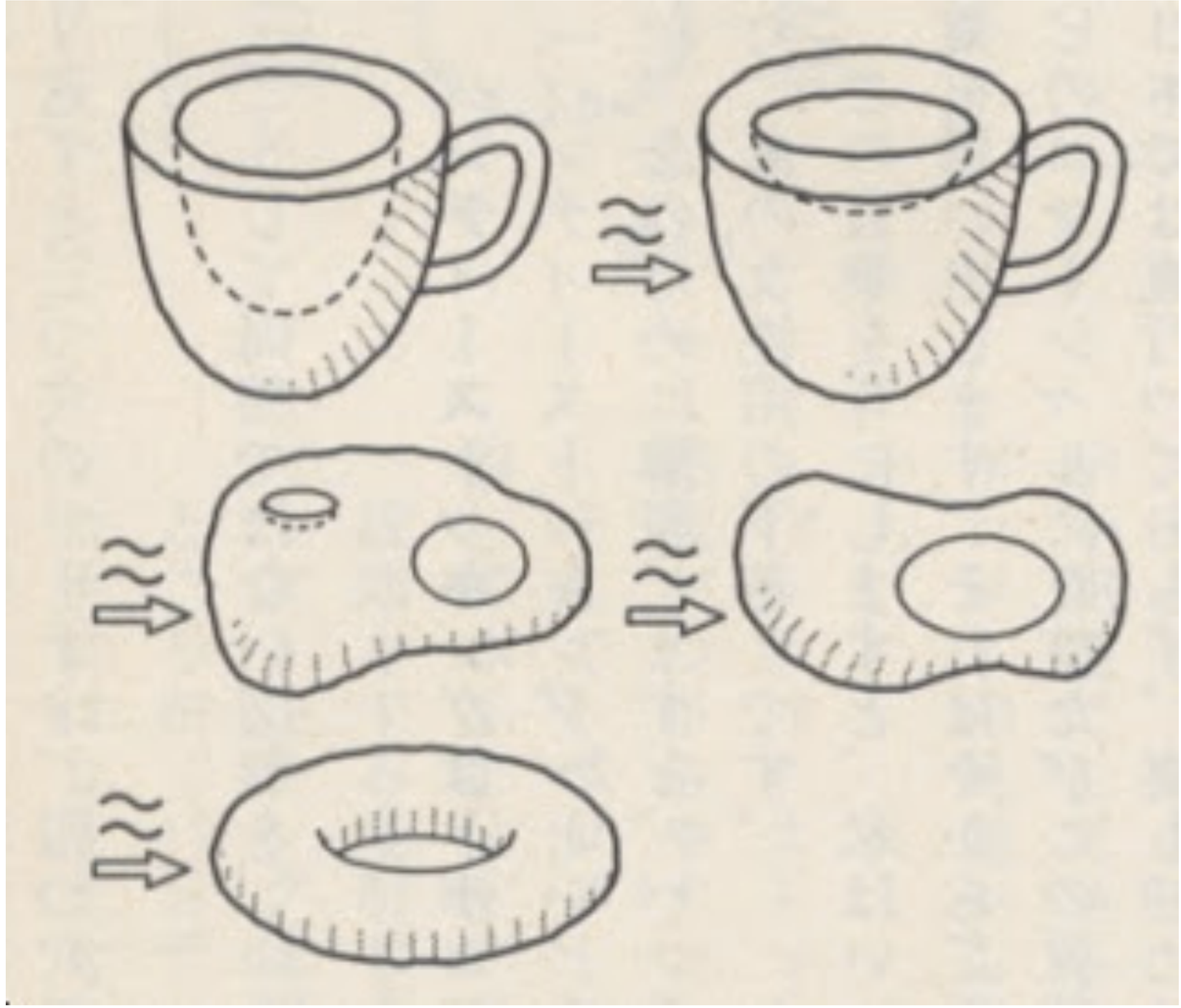
auf die Fläche gesetzt, sich nur entlang der Fläche bewegen kann, so kann dasselbe, wenn es einmal an der Aussenseite sich befindet, wie es sich auch bewegen mag, niemals an die Innenseite gelangen und umgekehrt. Ebenso kann man entweder die Aussenseite oder die Innenseite der Fläche für sich mit Farbe anstreichen. Doch nun kann man den Schlauch noch in ganz andrer Weise zusammenbiegen, indem man nämlich das eine Ende nach innen umstülpt, das andere dagegen durch die Wandung in das Innere hineinleitet und dann mit dem umgestülpten Ende vereinigt. v. Fig. 21. c.

Fig. 21.

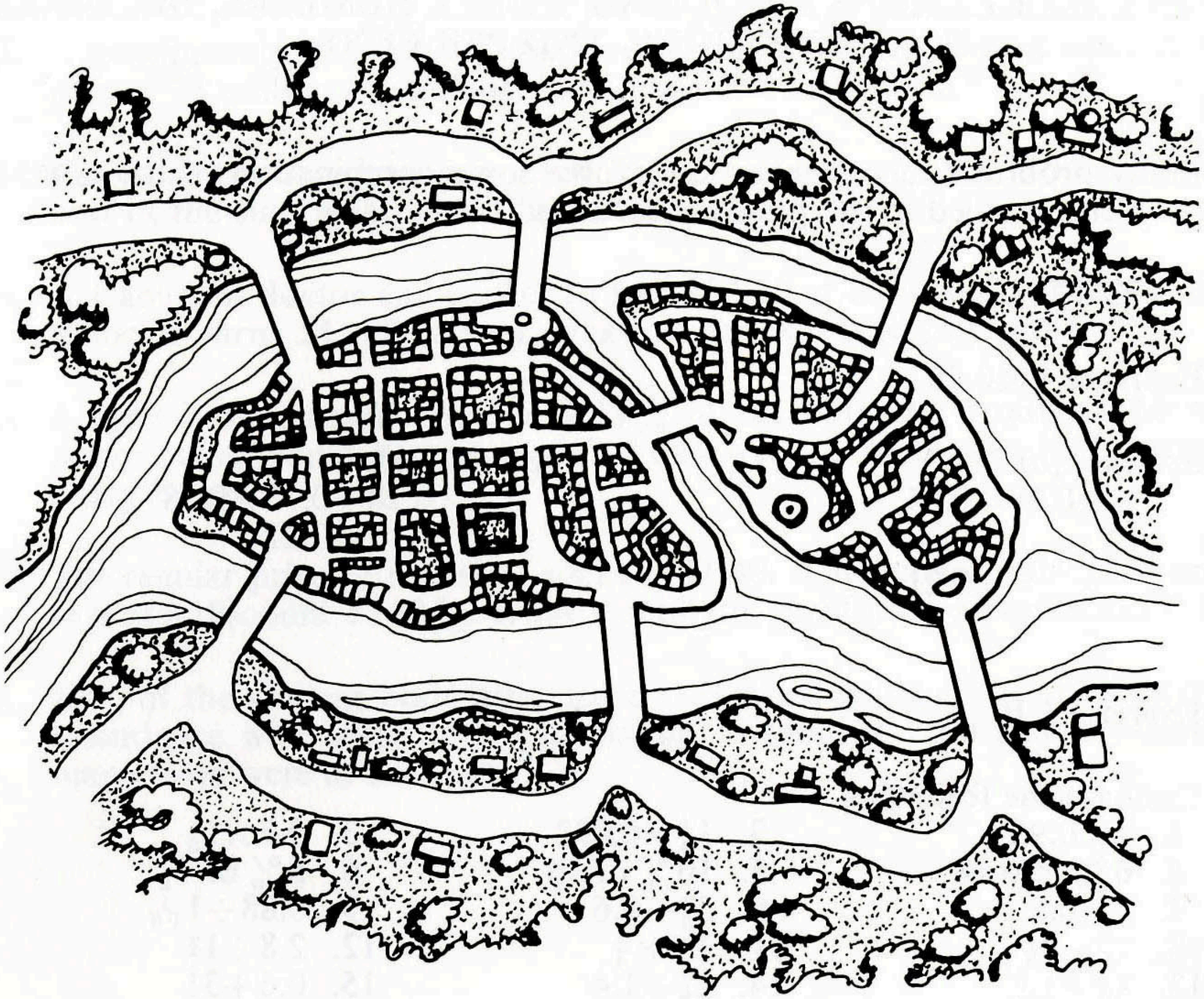
a) b) c)

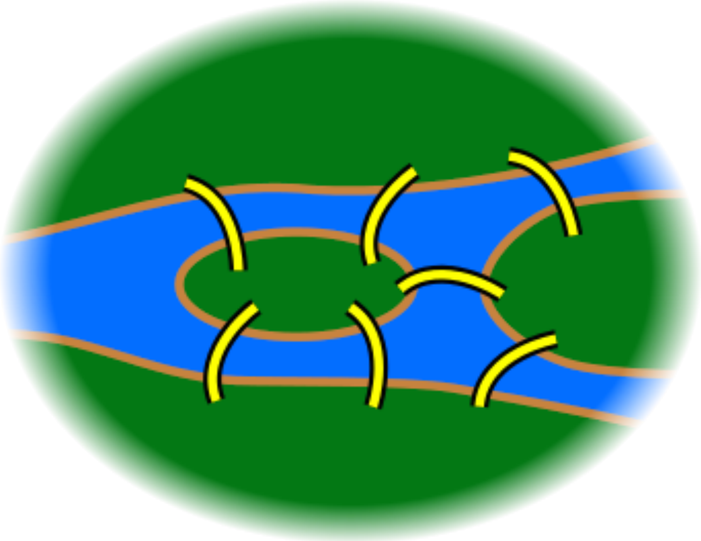
Acme

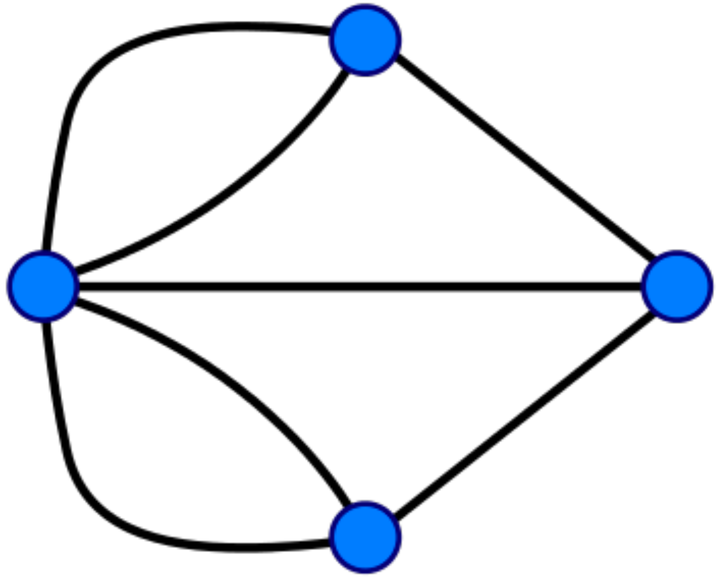
Acme diese Weise haben wir eine durchaus zusammenhängende Doppelfläche gewonnen, bei welcher eine Innen- und Aussenseite etwa durch besonderen farbigen Anstrich nicht mehr zu unterscheiden ist. Denken wir uns auf dieser Fläche ein zweidimensionales Wesen, so wird dies, indem es an seinen früheren Ort zurückgelangt, dabei sein eigener Antipode werden können, und es muss zweimal herumkriechen, ehe es in die Ausgangslage zurück.

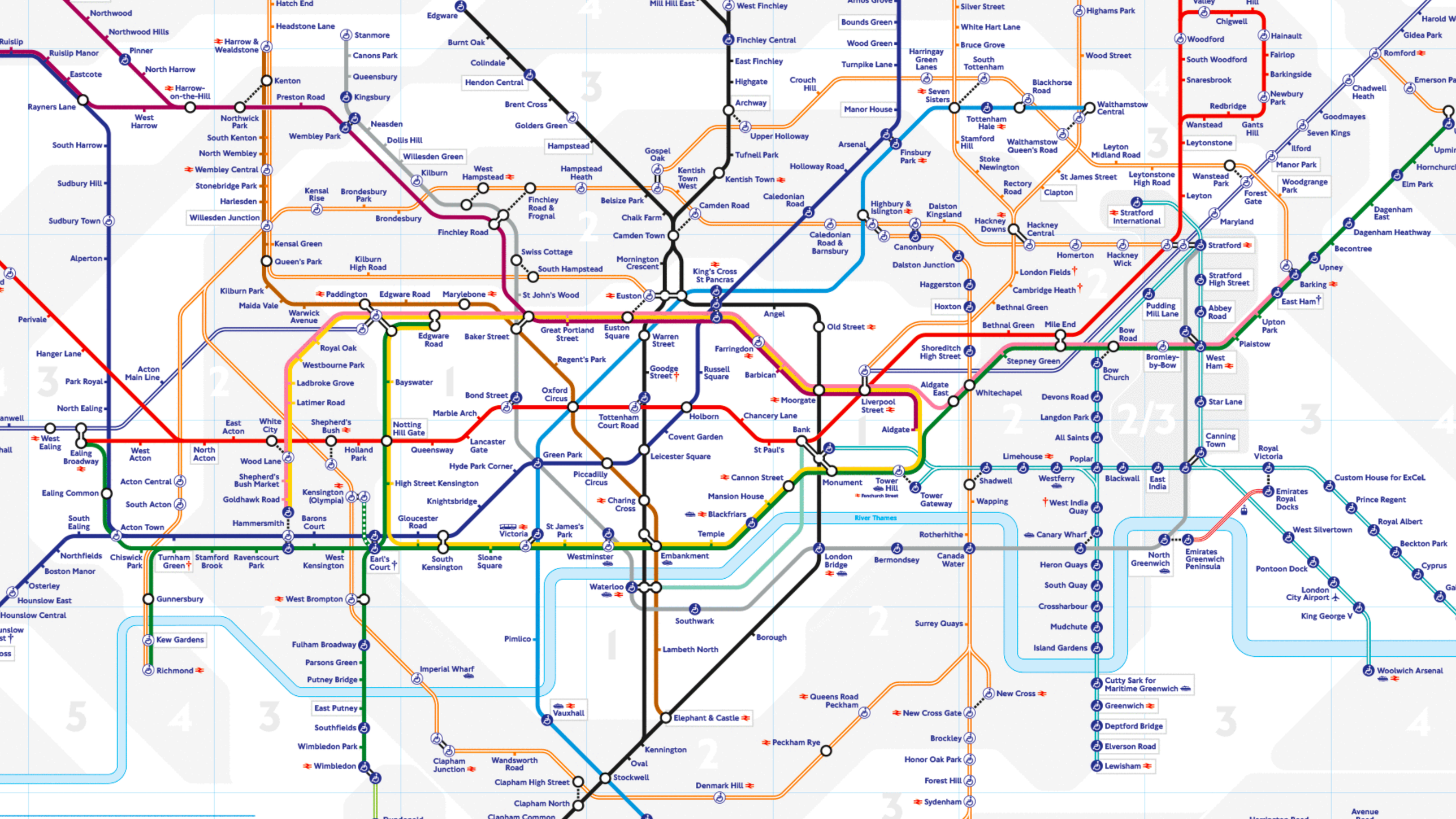


THE BRIDGES OF KONIGSBERG








Northwood
Northwood Hills
Pinner
North Harrow
Harrow-on-the-Hill
Ruislip
Ruislip Manor
Eastcote
Rayners Lane
West Harrow
South Harrow
Sudbury Hill
Sudbury Town
Alperton
Perivale
Hanger Lane
Park Royal
North Ealing
West Ealing
Ealing Broadway
Ealing Common
South Ealing
Acton Town
Acton Main Line
West Acton
North Acton
Acton Central
South Acton
Northfields
Boston Manor
Osterley
Hounslow East
Hounslow Central
Chiswick Park
Turnham Green
Stamford Brook
Ravenscourt Park
Hammersmith
Barons Court
West Kensington
Earl's Court
Gunnersbury
Kew Gardens
Richmond
Hatch End
Headstone Lane
Harrow & Wealdstone
Kenton
Preston Road
Northwick Park
South Kenton
North Wembley
Wembley Central
Stonebridge Park
Harlesden
Willesden Junction
Kensal Green
Queen's Park
Kilburn Park
Maida Vale
Kilburn High Road
Kensal Rise
Brondesbury Park
Brondesbury
Stanmore
Canons Park
Queensbury
Kingsbury
Wembley Park
Neasden
Dollis Hill
Willesden Green
Kilburn
West Hampstead
Finchley Road
Finchley Road & Frognal
Swiss Cottage
South Hampstead
Edgware
Burnt Oak
Colindale
Hendon Central
Brent Cross
Golders Green
Hampstead
Hampstead Heath
Belsize Park
Chalk Farm
Camden Town
Mornington Crescent
Euston
St John's Wood
Paddington
Edgware Road
Marylebone
Warwick Avenue
Royal Oak
Westbourne Park
Ladbroke Grove
Latimer Road
Bayswater
Notting Hill Gate
Queensway
Lancaster Gate
Marble Arch
Bond Street
Baker Street
Great Portland Street
Regent's Park
Oxford Circus
Green Park
Hyde Park Corner
Knightsbridge
High Street Kensington
Gloucester Road
South Kensington
Sloane Square
Victoria
St James's Park
Westminster
Pimlico
Vauxhall
Waterloo
Southwark
Lambeth North
Elephant & Castle
Kennington
Oval
Stockwell
Clapham Junction
Wandsworth Road
Clapham High Street
Clapham North
Clapham Common
Imperial Wharf
Fulham Broadway
Parsons Green
Putney Bridge
East Putney
Southfields
Wimbledon Park
Wimbledon
East Acton
White City
Wood Lane
Shepherd's Bush
Shepherd's Bush Market
Goldhawk Road
Kensington (Olympia)
Holland Park
Mill Hill East
West Finchley
Finchley Central
East Finchley
Highgate
Archway
Upper Holloway
Tufnell Park
Kentish Town
Kentish Town West
Gospel Oak
Camden Road
Caledonian Road
Holloway Road
Arsenal
Finsbury Park
Manor House
Turnpike Lane
Crouch Hill
Harringay Green Lanes
Seven Sisters
Bounds Green
Wood Green
Arnos Grove
Silver Street
White Hart Lane
Bruce Grove
South Tottenham
Tottenham Hale
Stamford Hill
Stoke Newington
Walthamstow Queen's Road
Blackhorse Road
Walthamstow Central
Highams Park
Wood Street
Leyton Midland Road
St James Street
Leytonstone High Road
Leytonstone
Wanstead
Wanstead Park
Leyton
Maryland
Stratford
Stratford International
Stratford High Street
Abbey Road
Pudding Mill Lane
Bow Road
Bromley-by-Bow
West Ham
Star Lane
Canning Town
Royal Victoria
Woodford
South Woodford
Snaresbrook
Redbridge
Chigwell
Hainault
Fairlop
Barkingside
Newbury Park
Gants Hill
Forest Gate
Manor Park
Ilford
Seven Kings
Goodmayes
Chadwell Heath
Romford
Gidea Park
Harold Wood
Emerson Park
Upminster
Hornchurch
Elm Park
Dagenham East
Dagenham Heathway
Becontree
Upney
Barking
East Ham
Upton Park
Plaistow
Woodgrange Park
Highbury & Islington
Dalston Kingsland
Canonbury
Dalston Junction
Haggerston
Hoxton
Hackney Downs
Hackney Central
Hackney Wick
Homerton
London Fields
Cambridge Heath
Bethnal Green
Mile End
Caledonian Road & Barnsbury
King's Cross St Pancras
Angel
Old Street
Farringdon
Barbican
Moorgate
Liverpool Street
Aldgate
Aldgate East
Shoreditch High Street
Whitechapel
Stepney Green
Bow Church
Devons Road
Langdon Park
All Saints
Poplar
Limehouse
Westferry
Blackwall
East India
Shadwell
Wapping
Rotherhithe
Canada Water
Canary Wharf
West India Quay
Heron Quays
South Quay
Crossharbour
Mudchute
Island Gardens
Cutty Sark for Maritime Greenwich
Greenwich
Deptford Bridge
Elverson Road
Lewisham
North Greenwich
Emirates Greenwich Peninsula
Emirates Royal Docks
Custom House for ExCeL
Prince Regent
Royal Albert
Beckton Park
Cyprus
West Silvertown
Pontoon Dock
London City Airport
King George V
Woolwich Arsenal
Surrey Quays
New Cross
New Cross Gate
Queens Road Peckham
Peckham Rye
Brockley
Honor Oak Park
Forest Hill
Sydenham
Denmark Hill
Borough
London Bridge
Bermondsey
Tower Hill
Tower Gateway
Monument
Bank
St Paul's
Cannon Street
Mansion House
Blackfriars
Temple
Embankment
Charing Cross
Leicester Square
Covent Garden
Holborn
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Russell Square
Tottenham Court Road
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Why are we talking about it?

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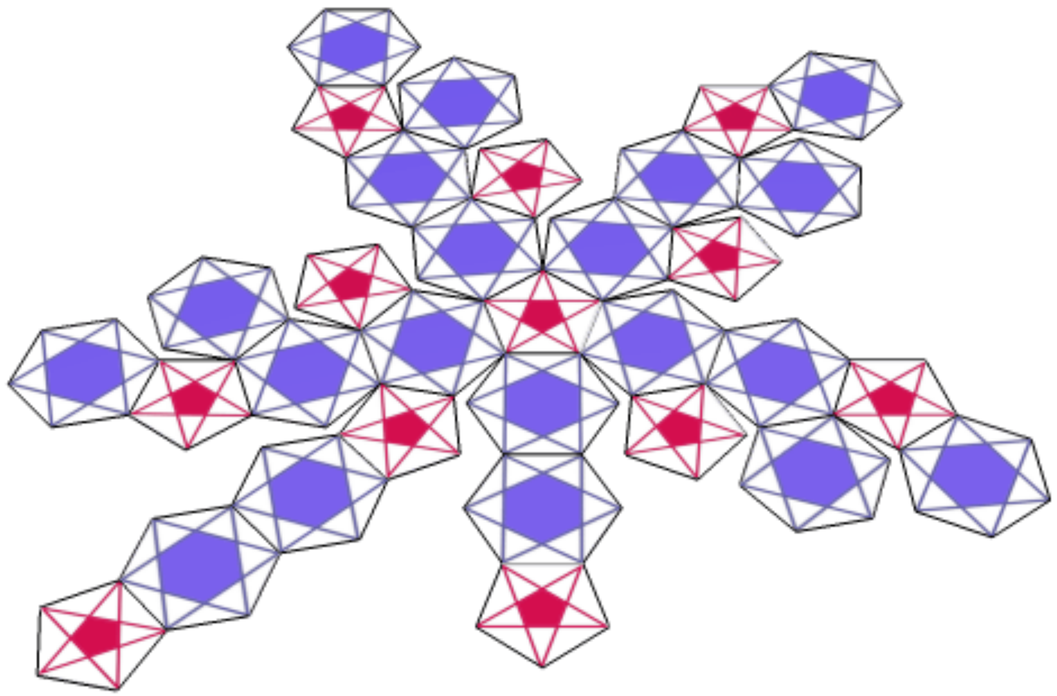

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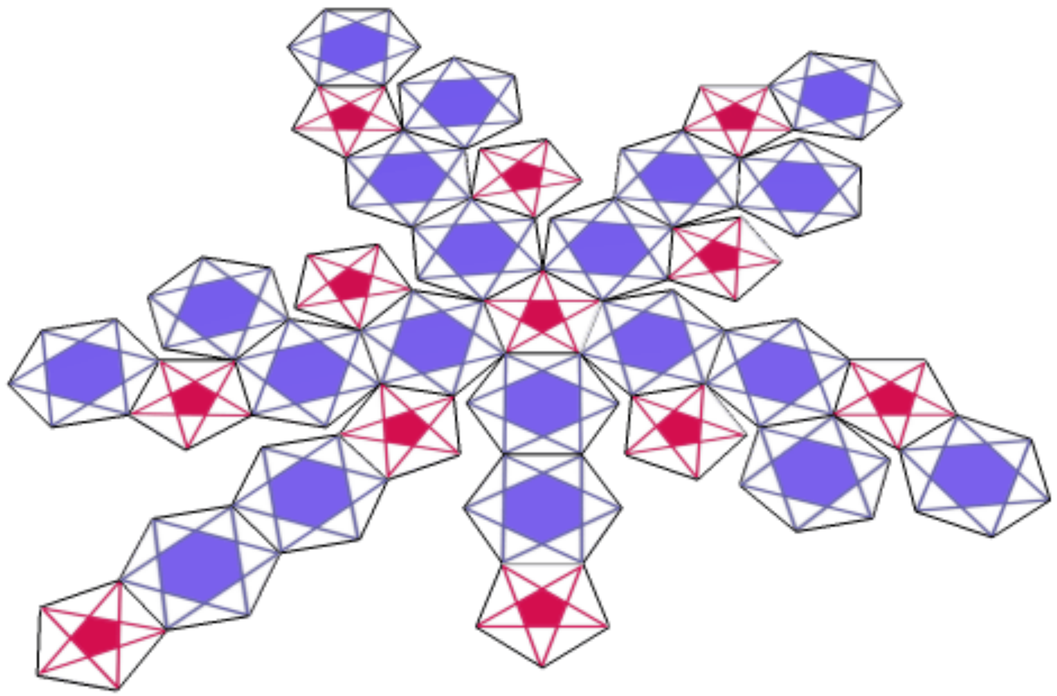

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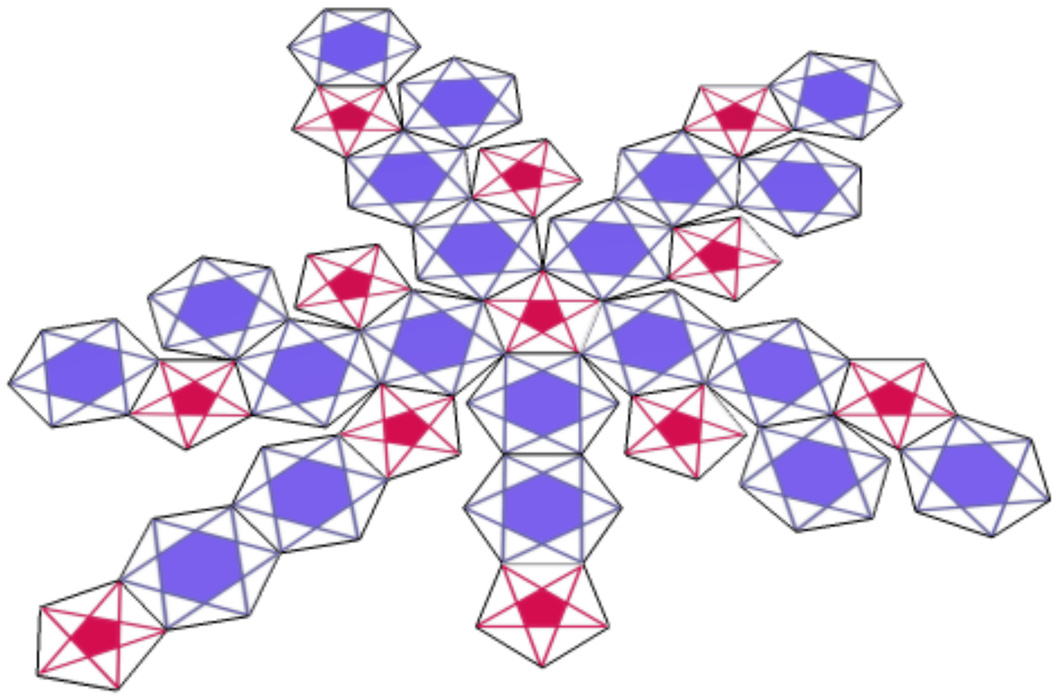
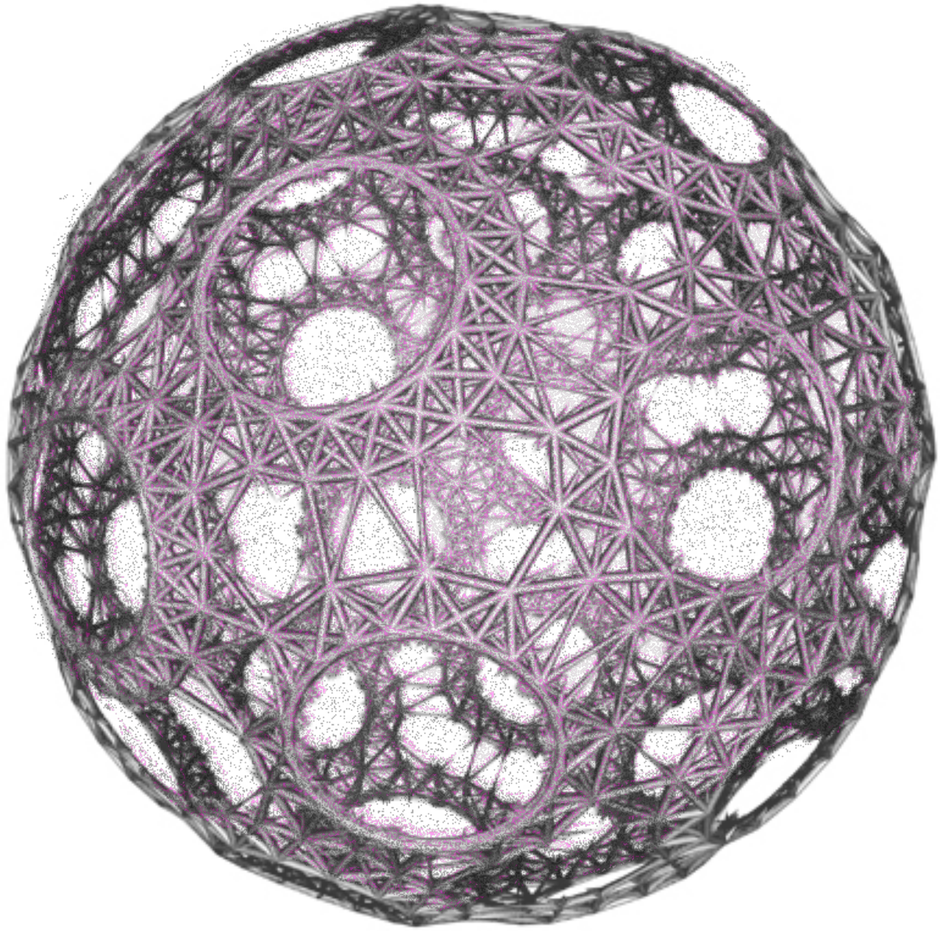
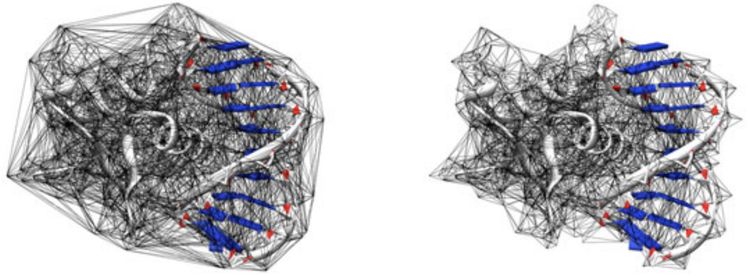


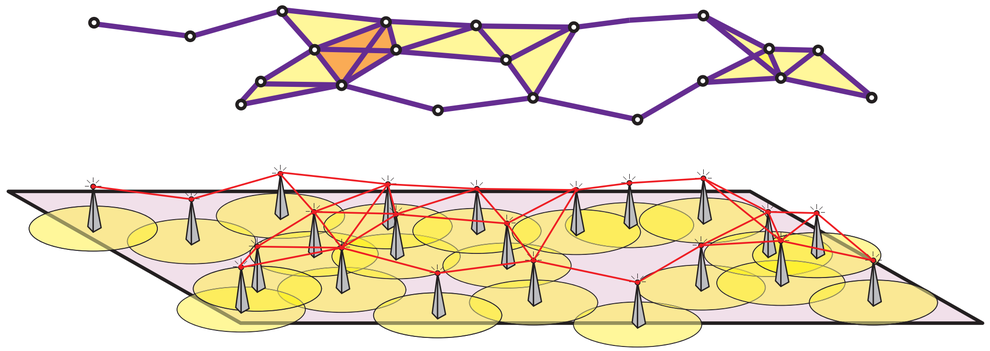


Topology in complex systems

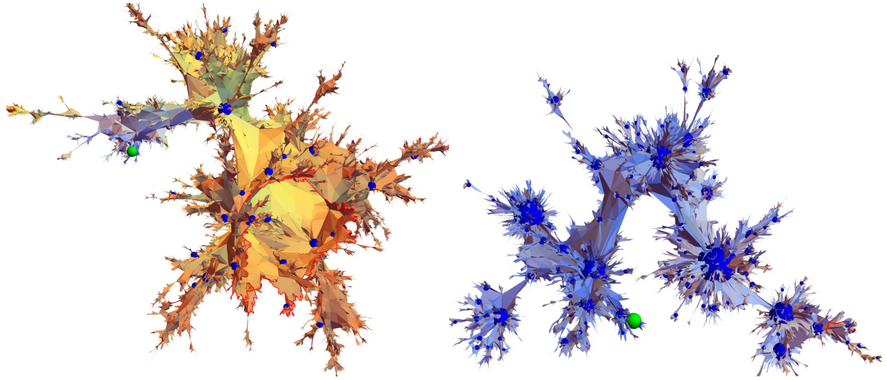
Protein folding

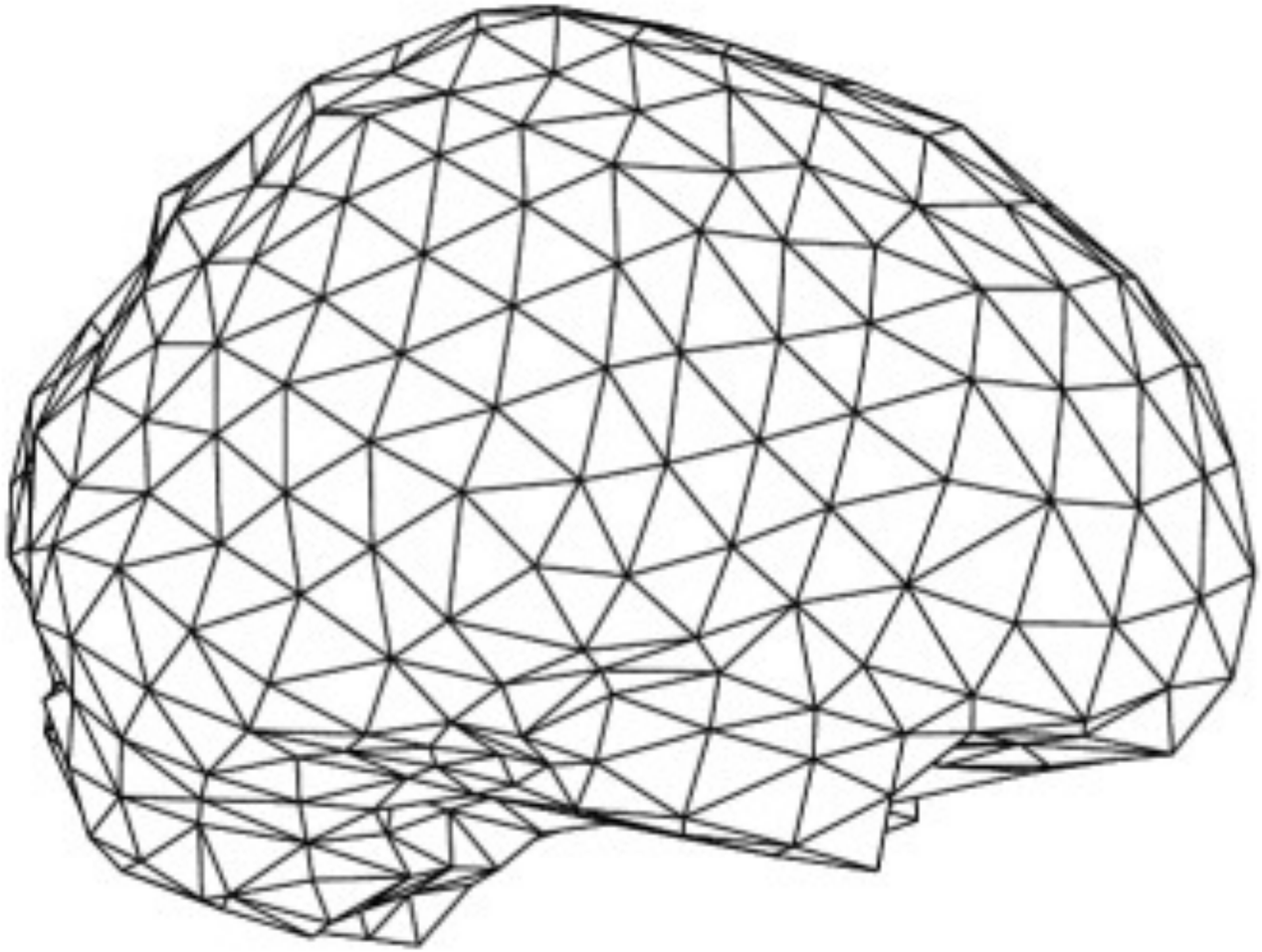


Sensor networks



Quantum gravity





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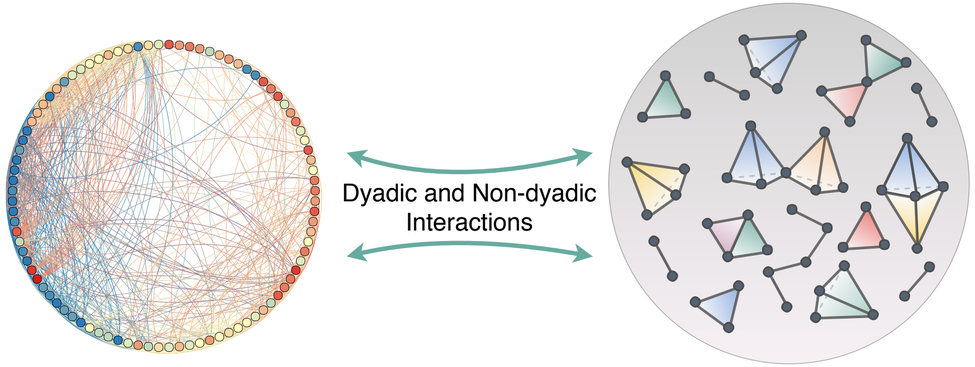
1. **Higher-order interactions:**
    1. Paradigmatic example: collaboration
    2. complex contagion / local environment
    3. gene-gene interactions
    4. Some type of neuronal interactions



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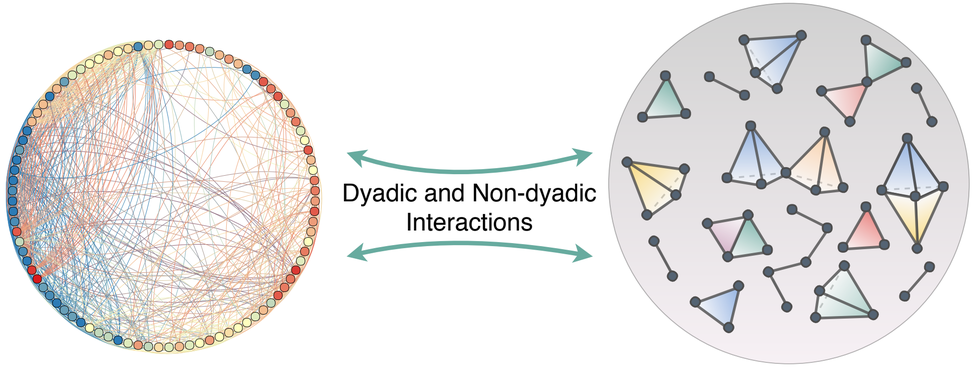
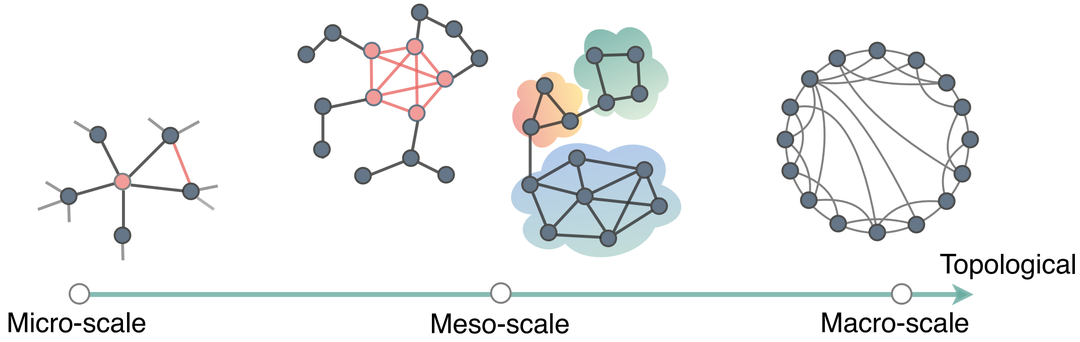


2. **Shapes / Mesoscale structures**
    1. Organisation on intermediate scales
    2. Non-local features



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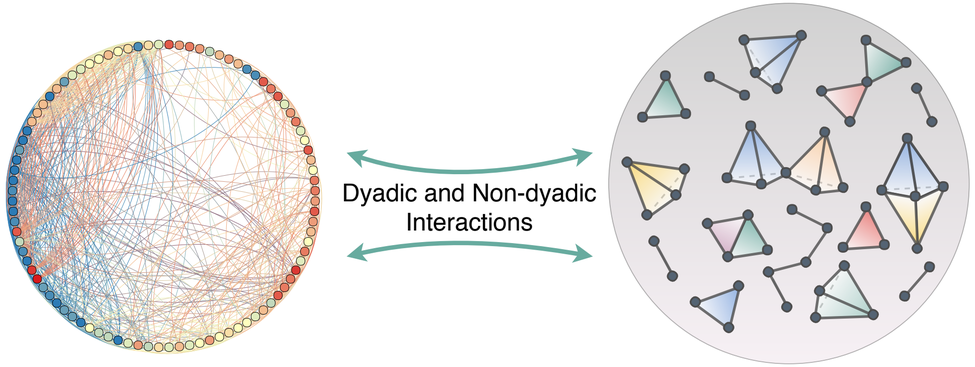

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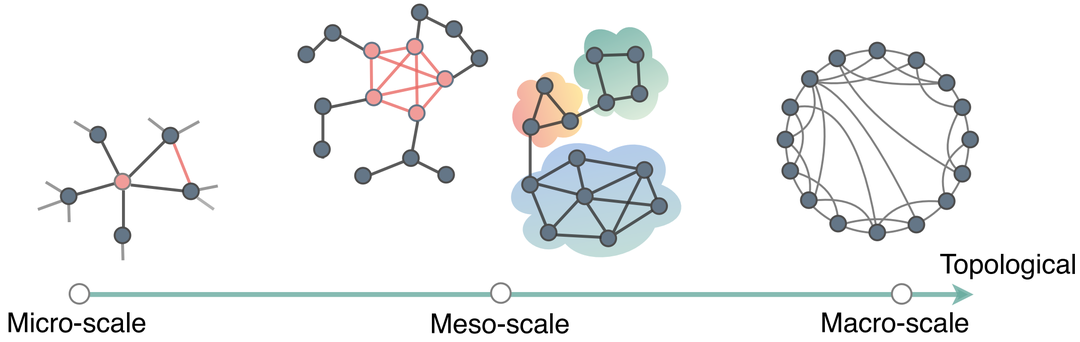

3. **General comparison of spaces**
    1. Distance manifold to manifold
    2. Compare networks with different structures

What does it mean in practice?

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1. **(Persistent) homology**
    1. Multiscale description of a network/space
    2. Complementary to communities/blocks
    3. Categorical foundation

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    1. Configuration models (SCM, ERSC)
    2. Generative models (Network geo+flavour)
    3. Dynamics on/off models (SAD)

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TDA

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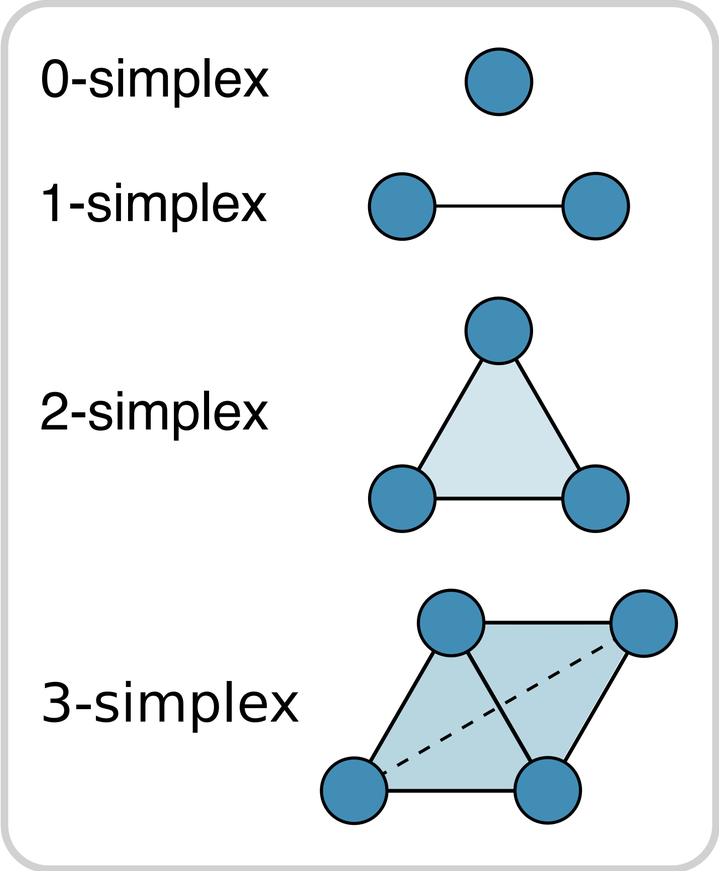
"Netsci"

Back to basics

Back to basics: simplices

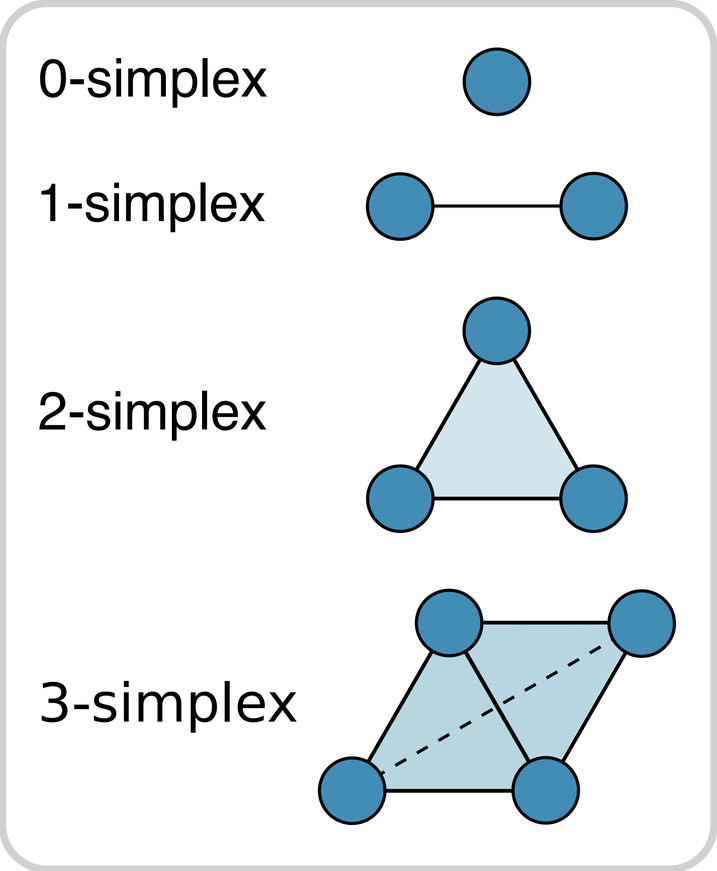
d-dimensional
group interactions



Back to basics: simplices

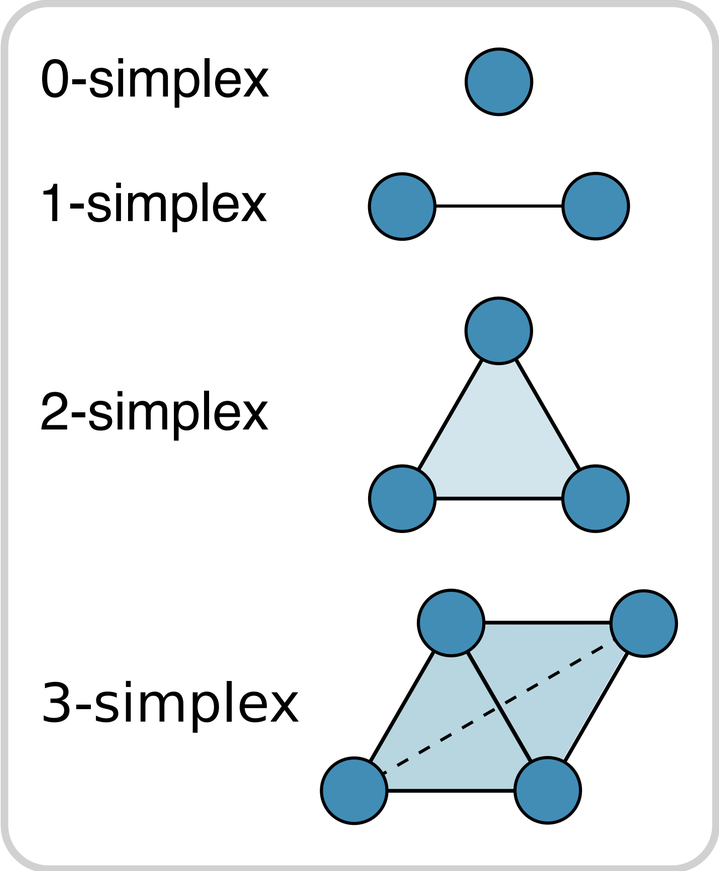
Definition

A $n-$dimensional *SIMPLEX* in $\mathbb{R}^m$ is the convex hull of $n+1$ points in general position in $\mathbb{R}^m$. $(m \geq n)$

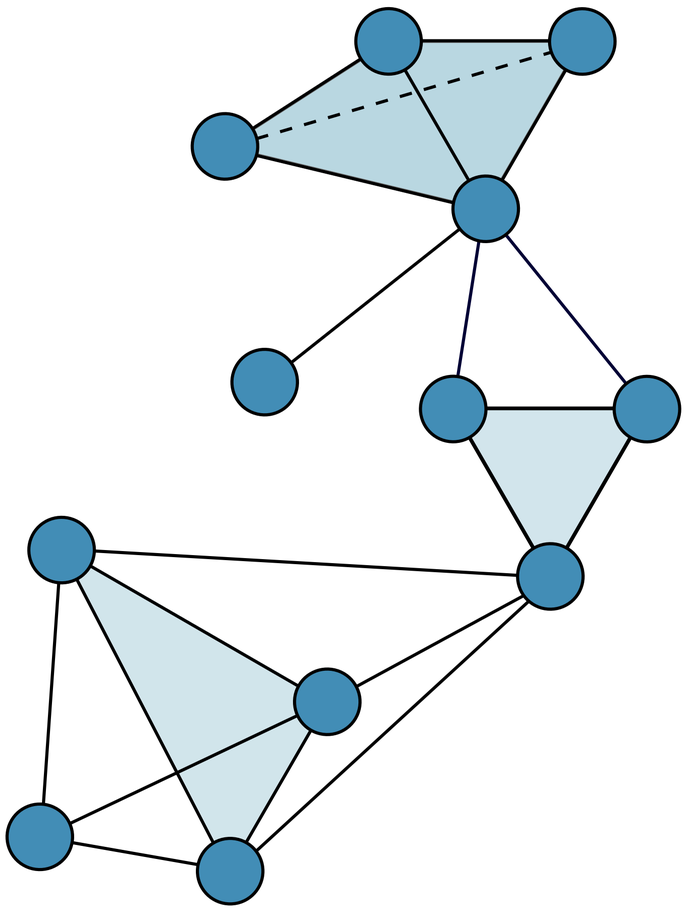


Back to basics: simplicial complexes

d-dimensional
group interactions

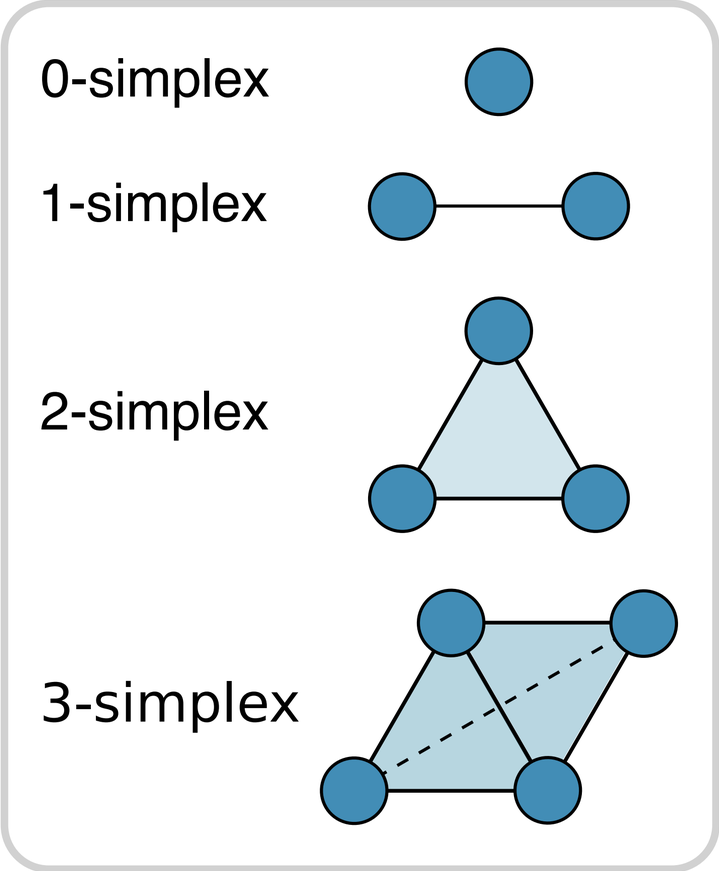


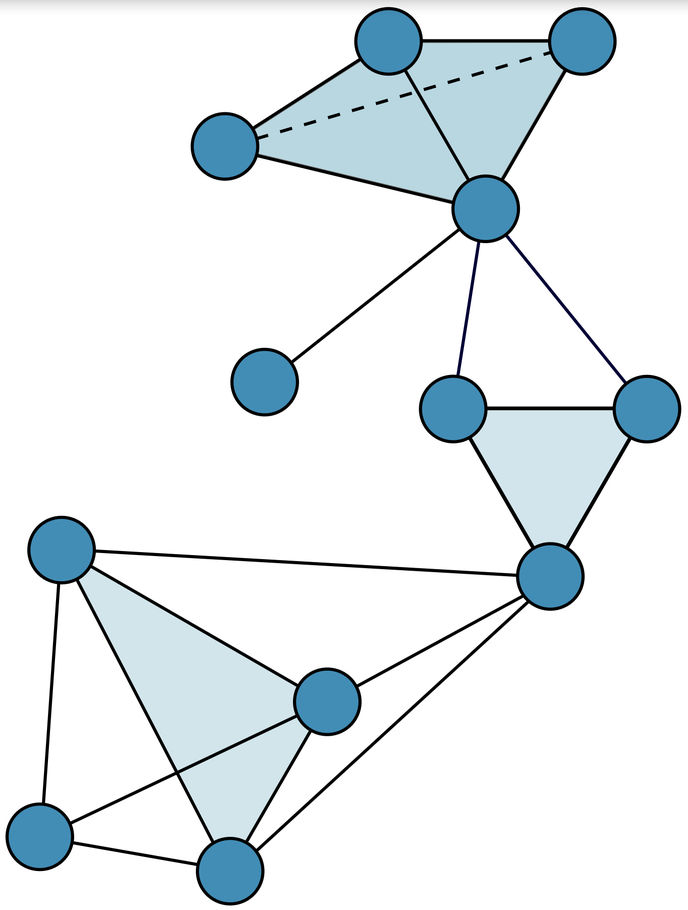
Social structure:
simplicial complex



Back to basics: simplicial complexes

A simplicial complex $\mathscr{K}$ on a given set of vertices $\mathscr{V}$, with $|\mathscr{V}| = N$, is a collection of simples with the extra requirement that if a simplex $\sigma \in \mathscr{K}$, then all the sub-simplices $\nu \subset \sigma$ built from the subset of σ are also contained in $\mathscr{K}$.





Simplicial complex

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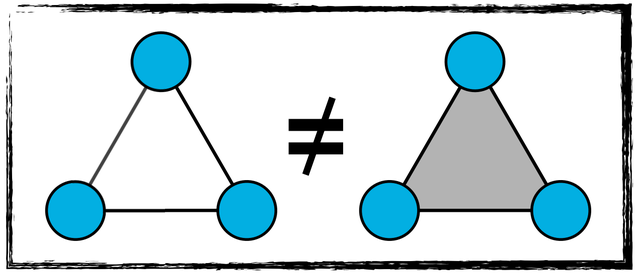
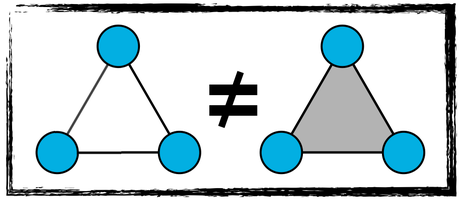
Notice that



Simplicial complex

Interaction: co-authorship



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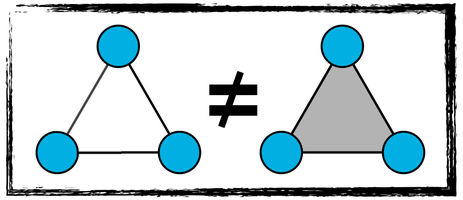

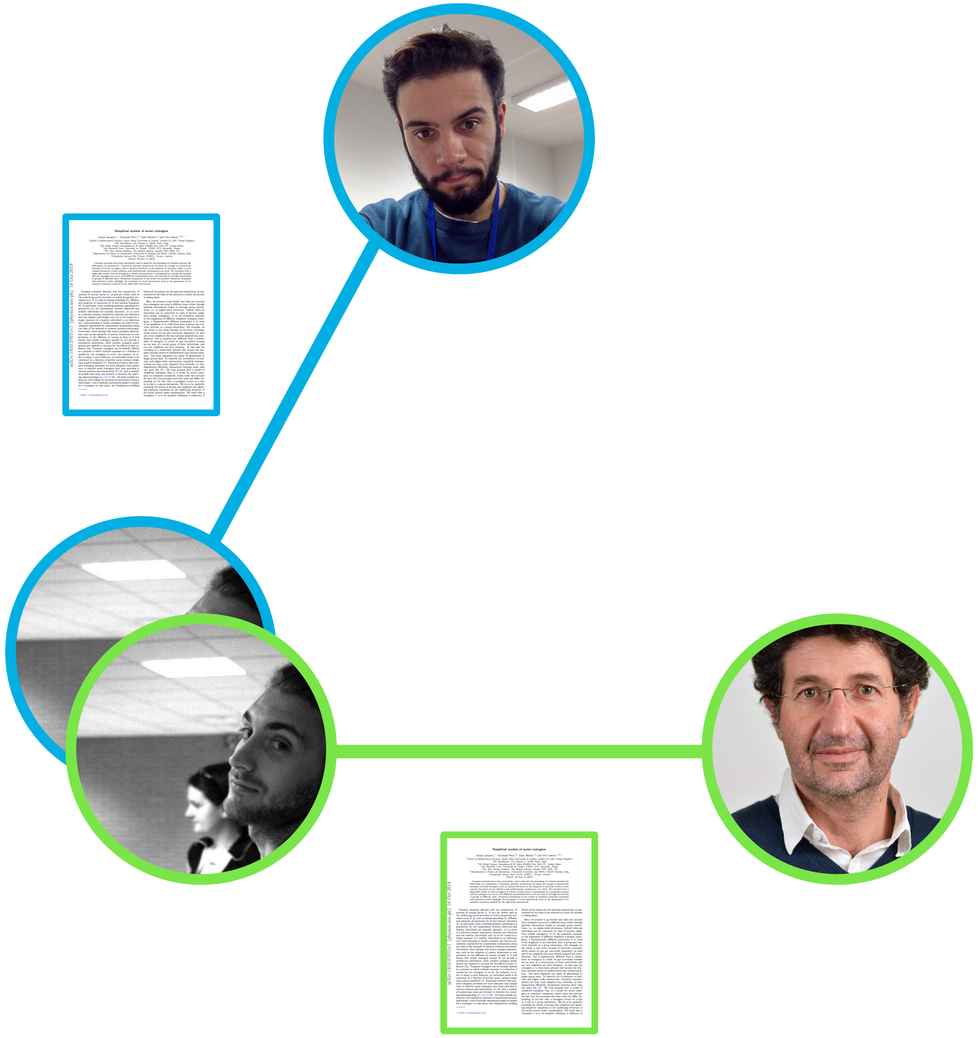

Simplicial complex

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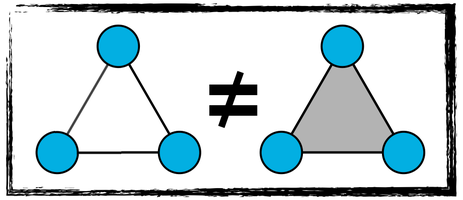

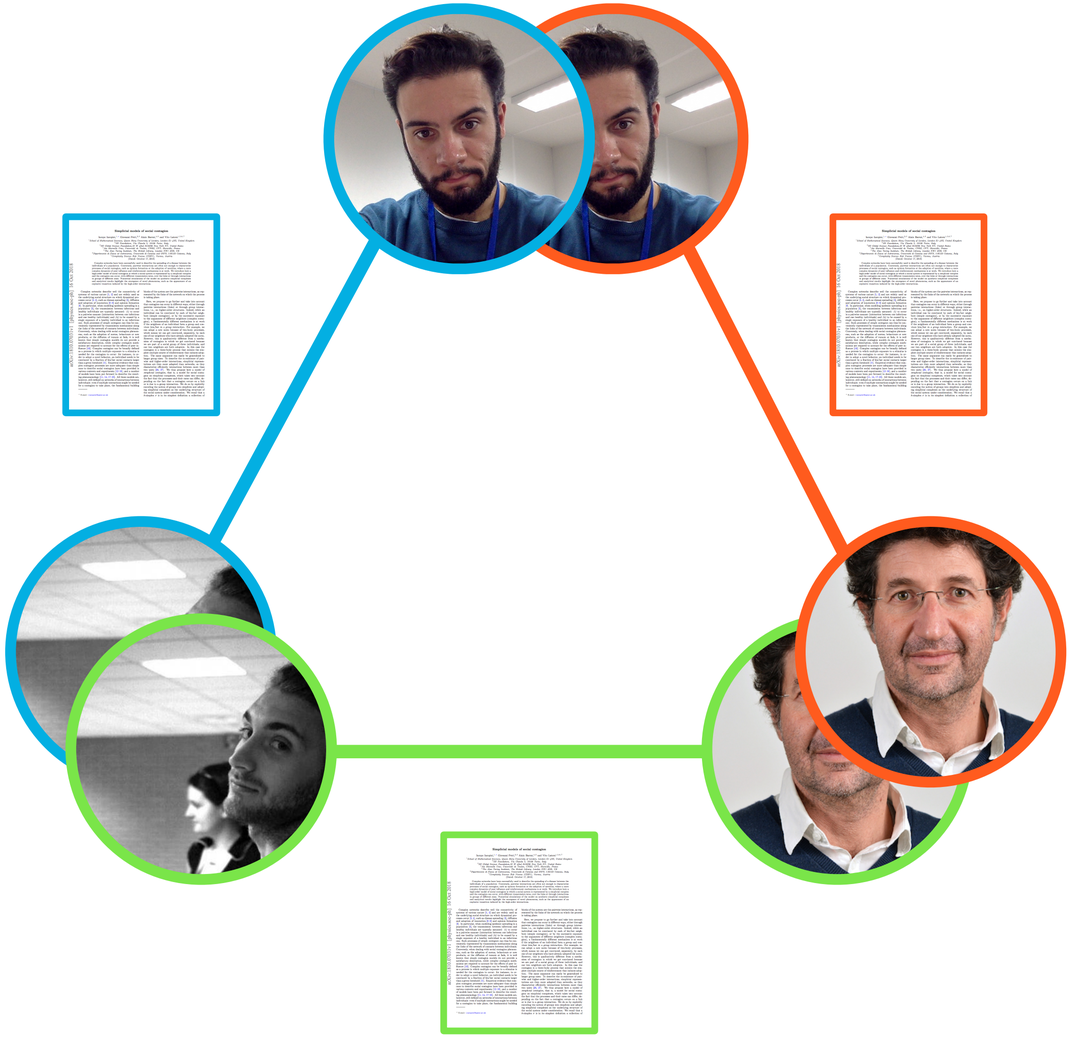

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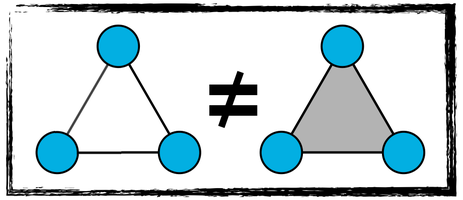

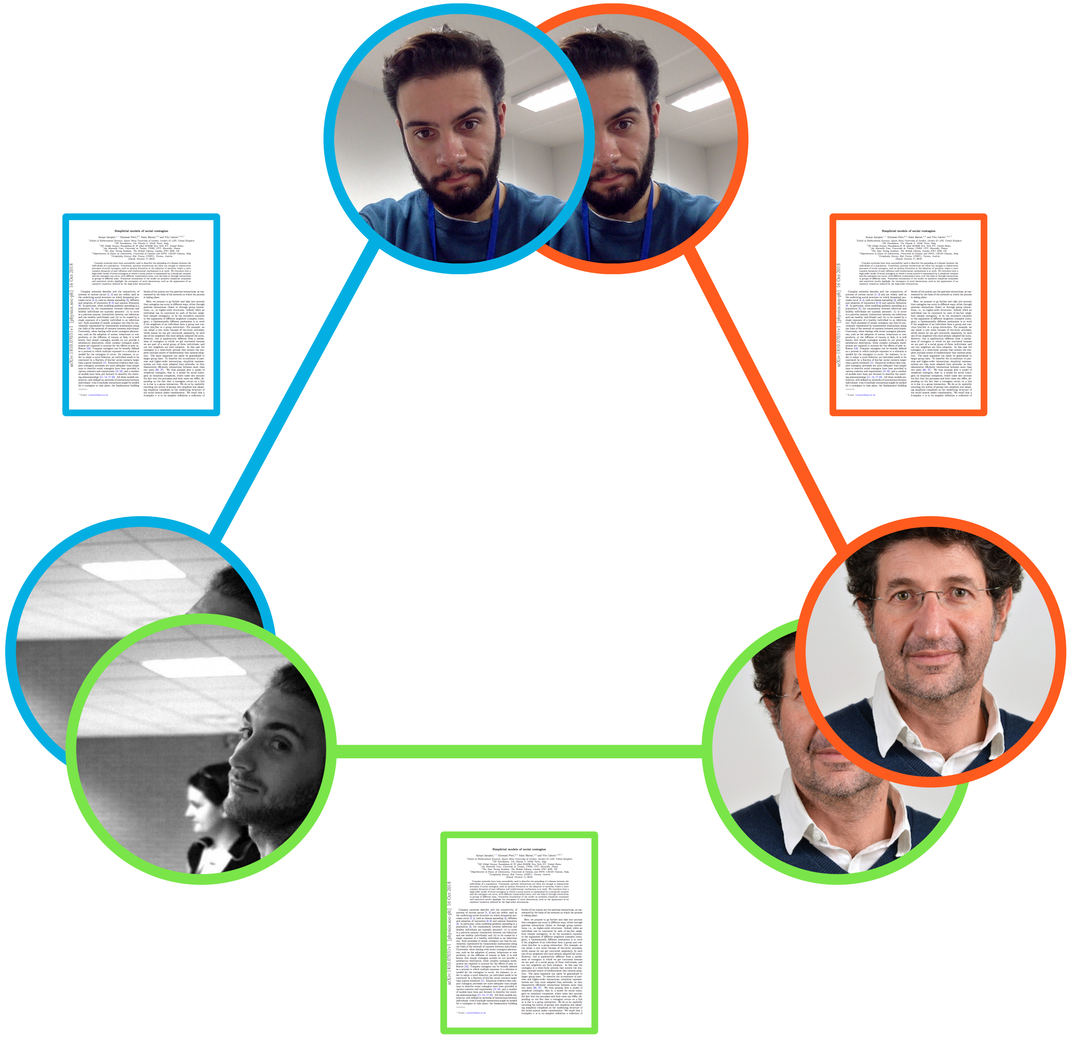

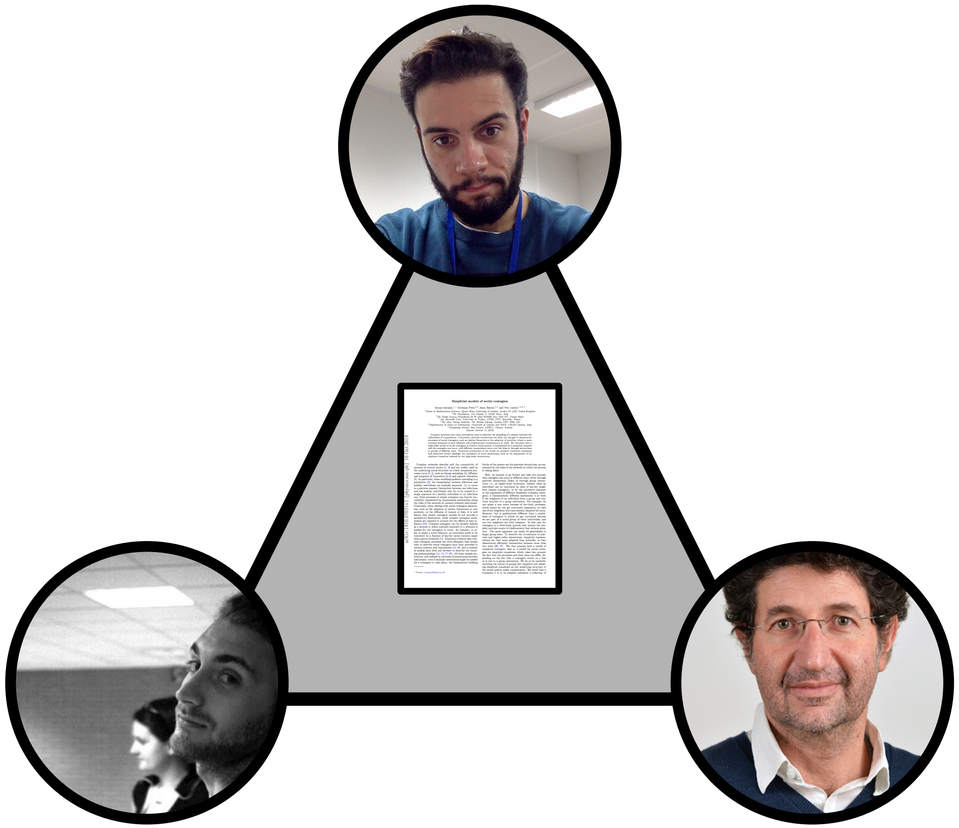

Back to basics: degrees

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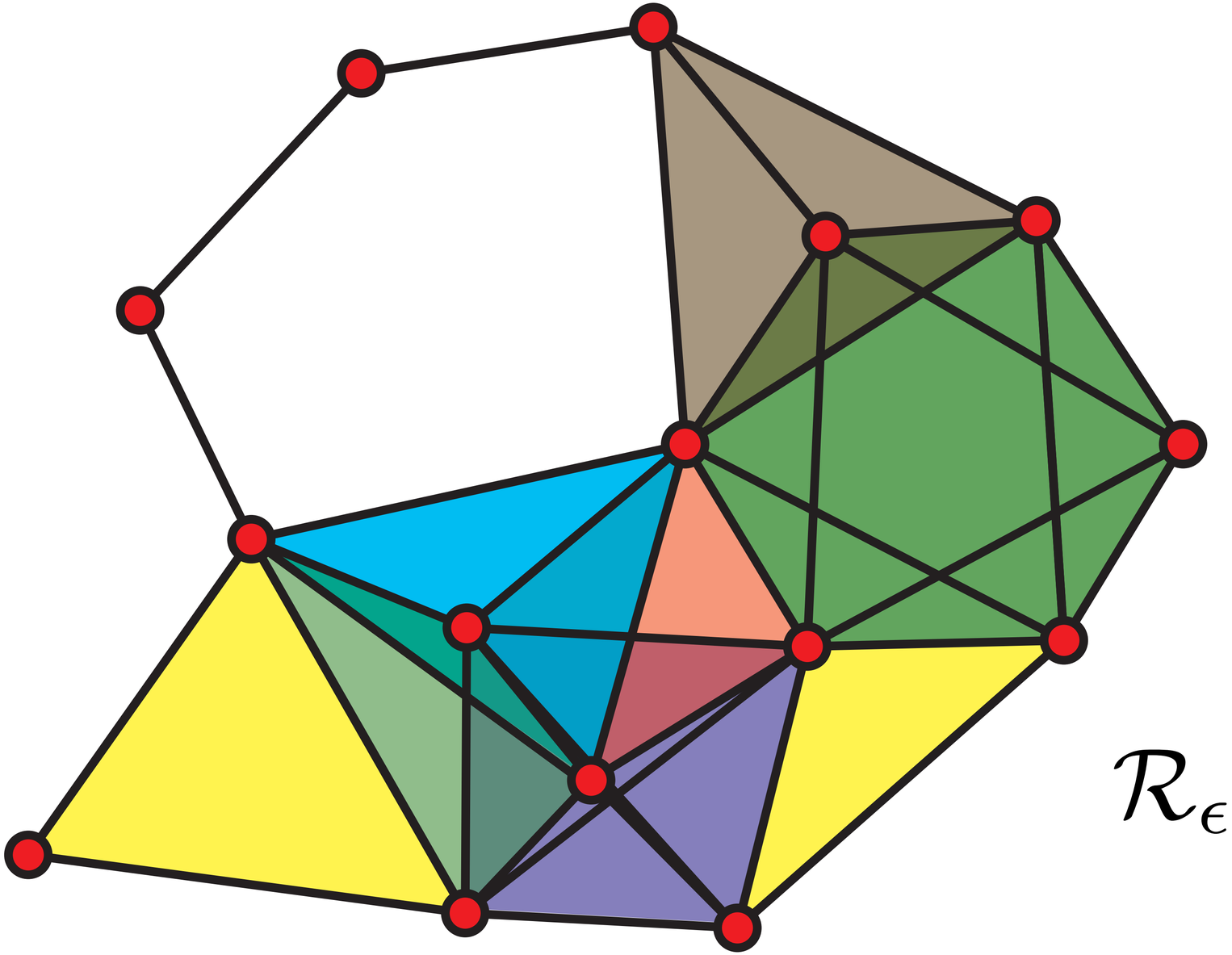
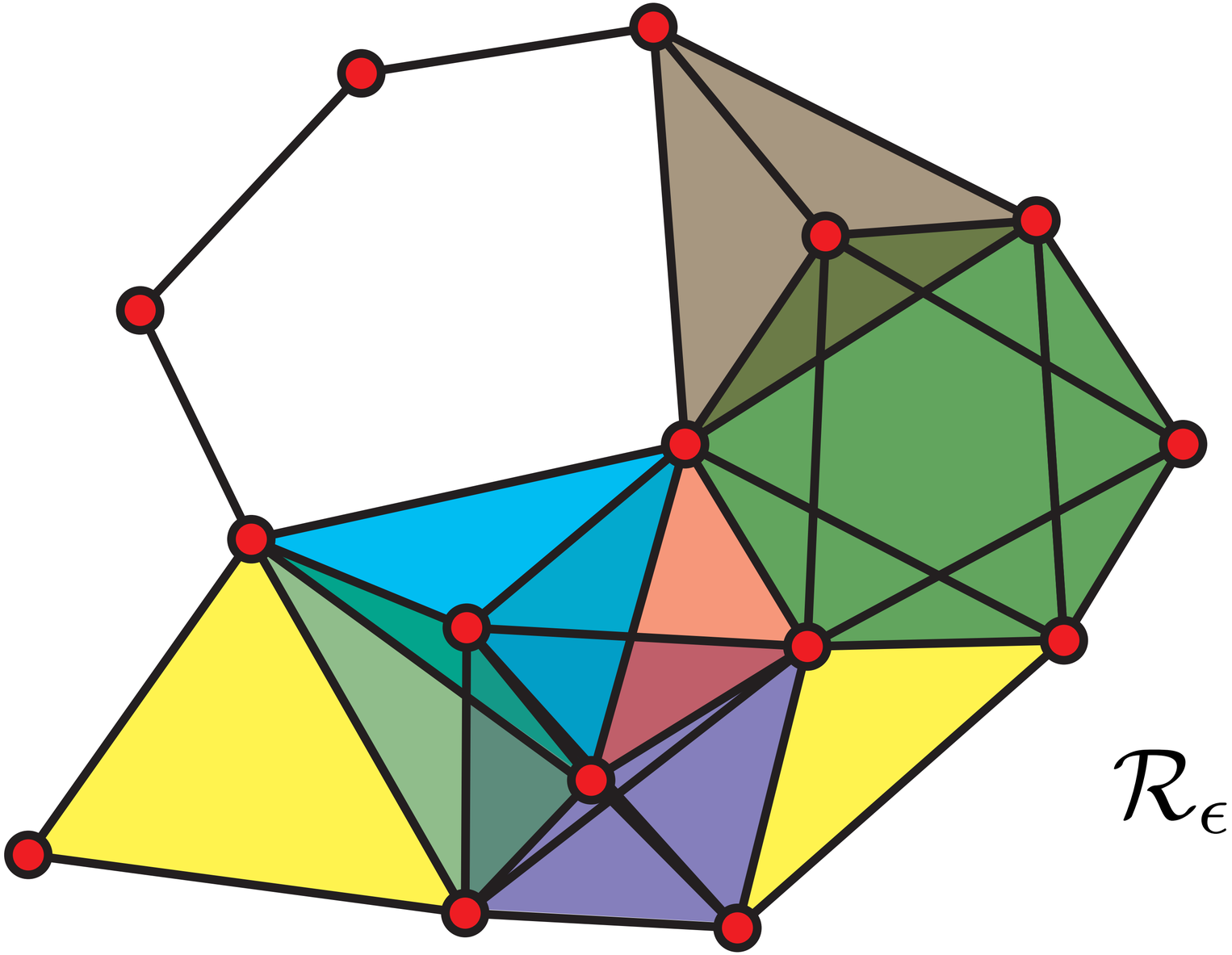


$\mathcal{R}_\epsilon$

Back to basics: degrees



$$a_\alpha = \begin{cases} 1 & \text{if} \quad \alpha \in \mathcal{S}_{d,d} \\ 0 & \quad \text{otherwise} \end{cases} .$$

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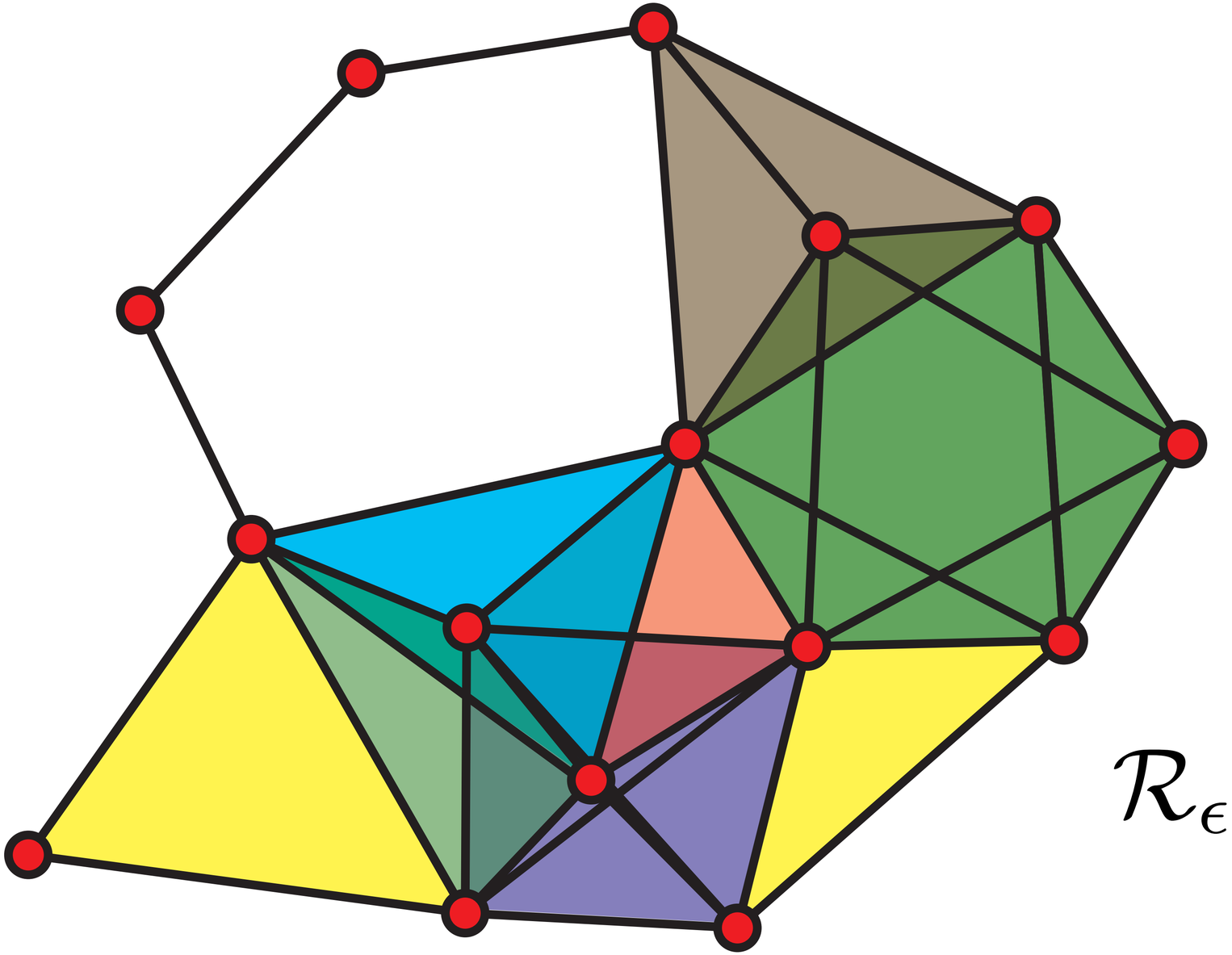

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Generalized simplicial degree (Courney-Bianconi 2016)

$$k_{d,\delta}(\alpha) = \sum_{\alpha' \in \mathcal{Q}_d(N) | \alpha' \supseteq \alpha} a_{\alpha'} .$$

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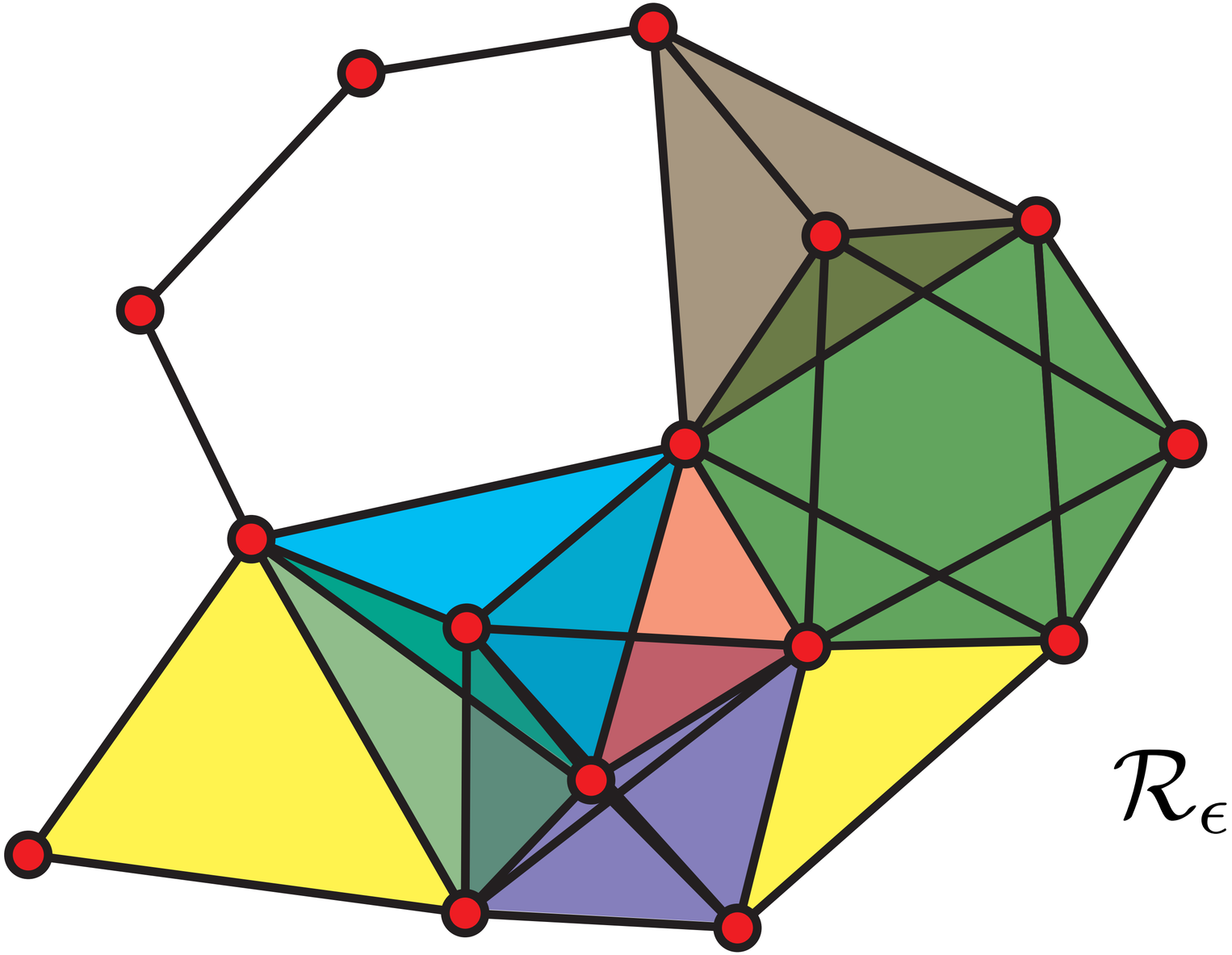

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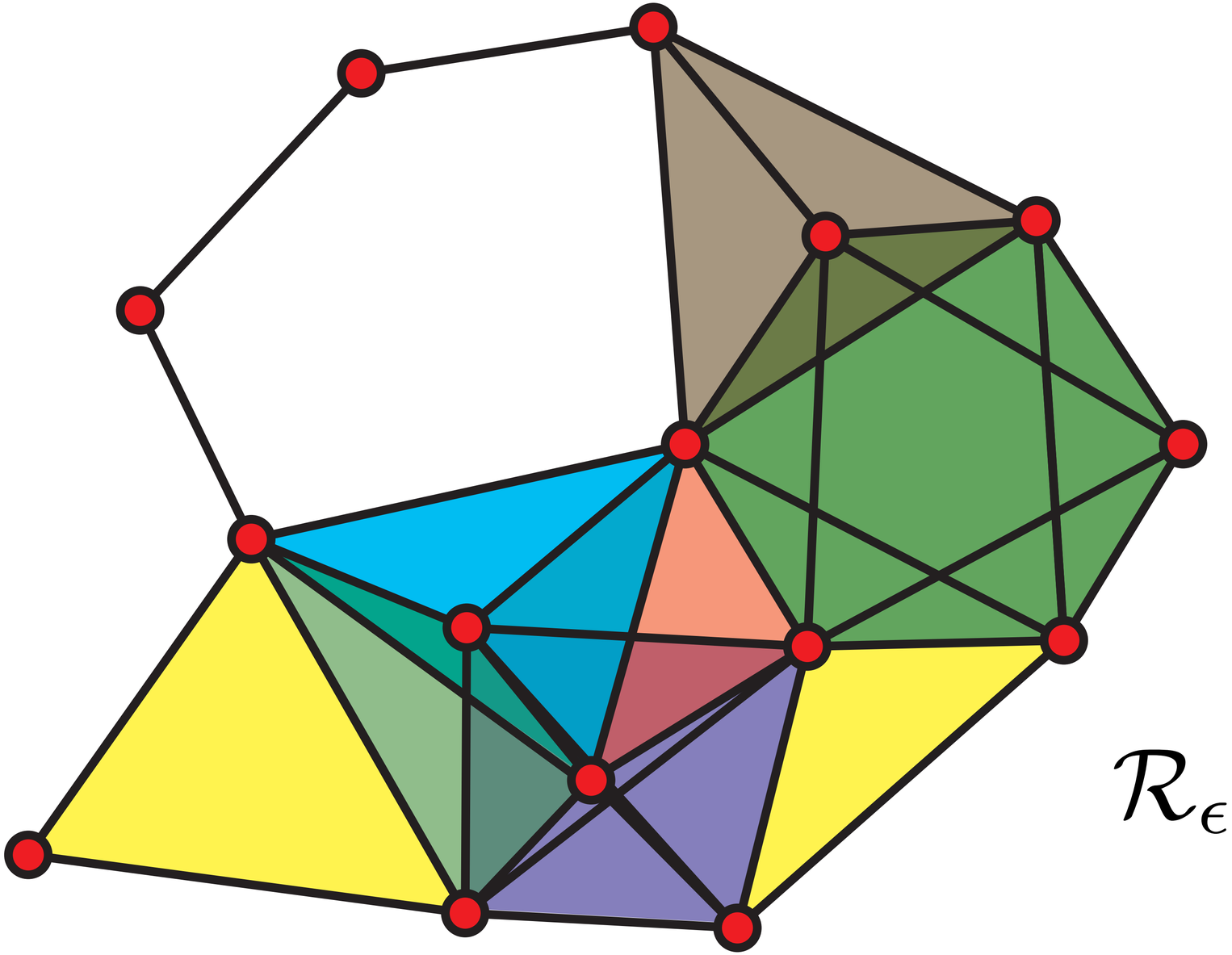
Back to basics: degrees



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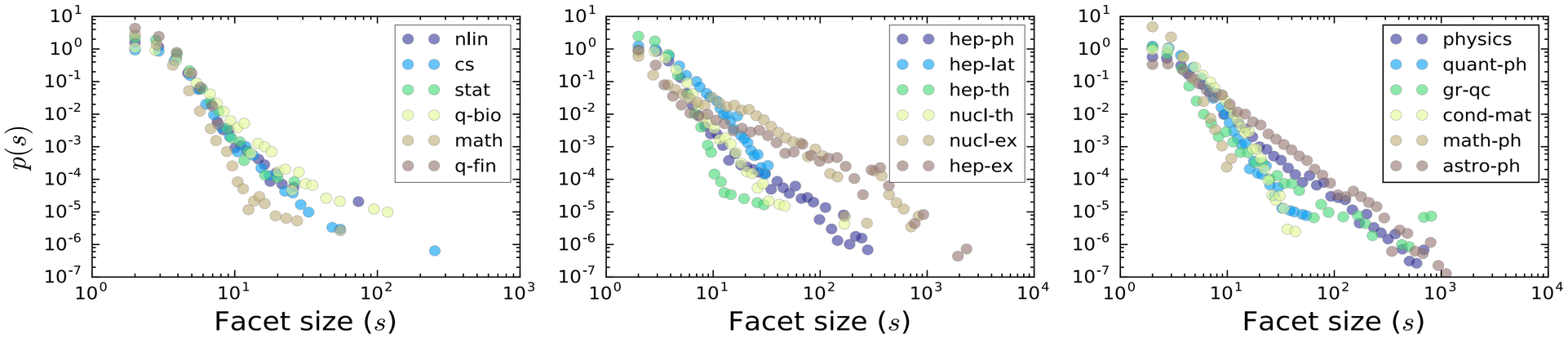
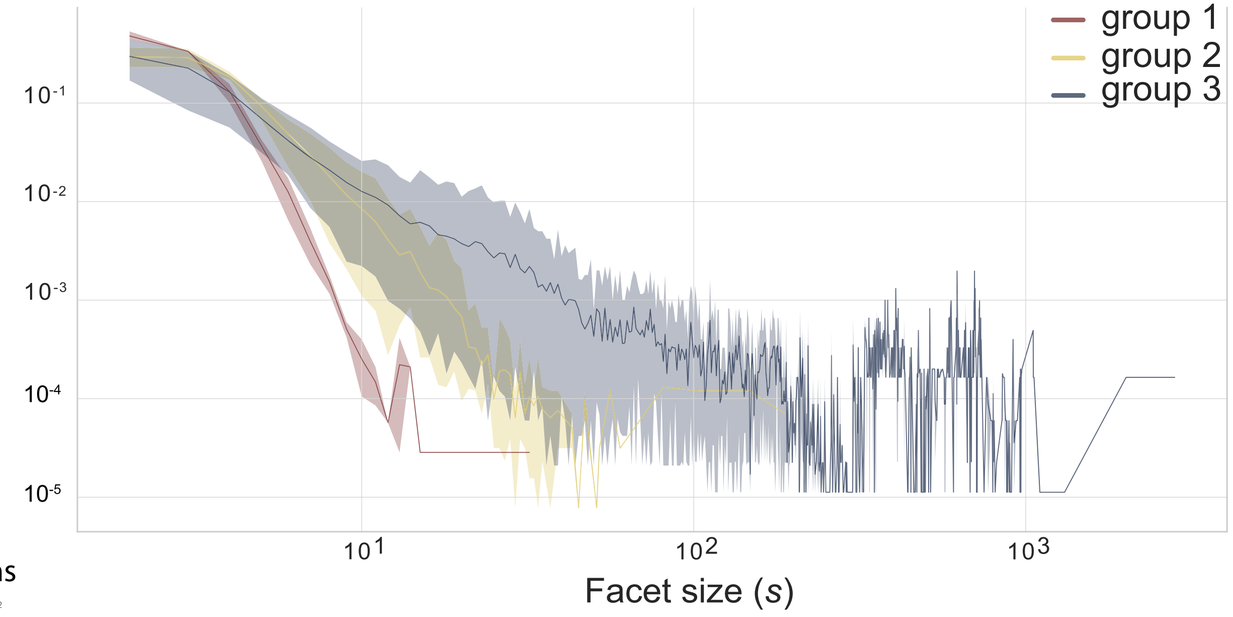
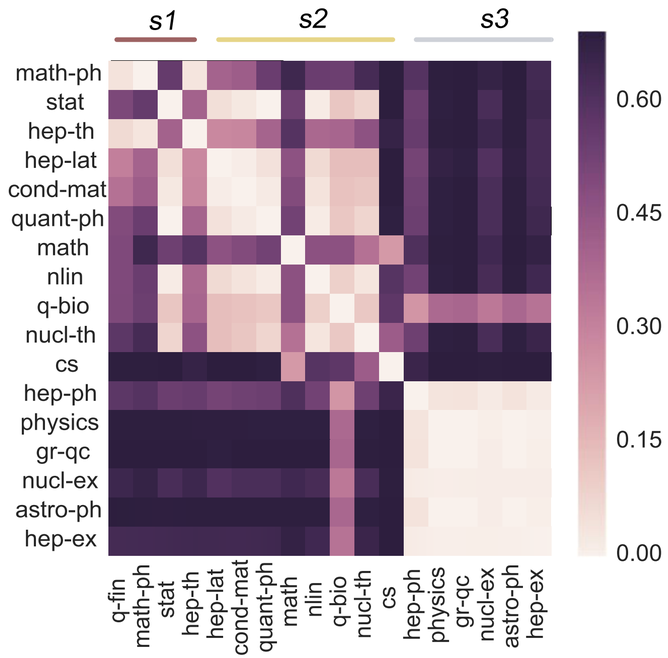
Pure simplicial degree ("Facet degree") (Young, Vaccarino, Petri, Patania 2017)

$$\tilde{k}_{d,\delta}(\alpha) = \sum_{\alpha' \in \mathcal{F} | \alpha \subset \alpha'} a_{\alpha'}$$

Are high-order interactions meaningful?







The shape of collaborations

Alice Patania[1,2*], Giovanni Petri[1] and Francesco Vaccarino[1,2]

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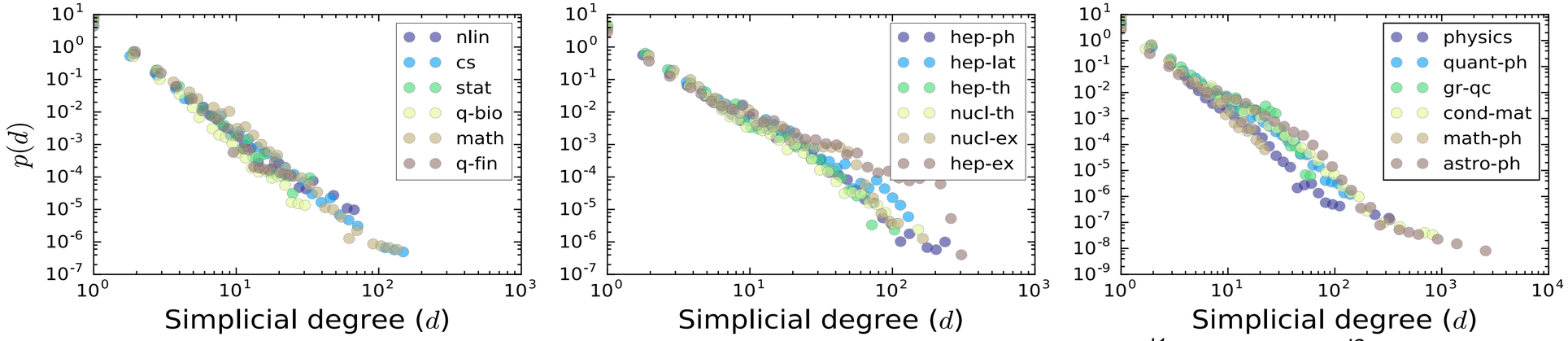

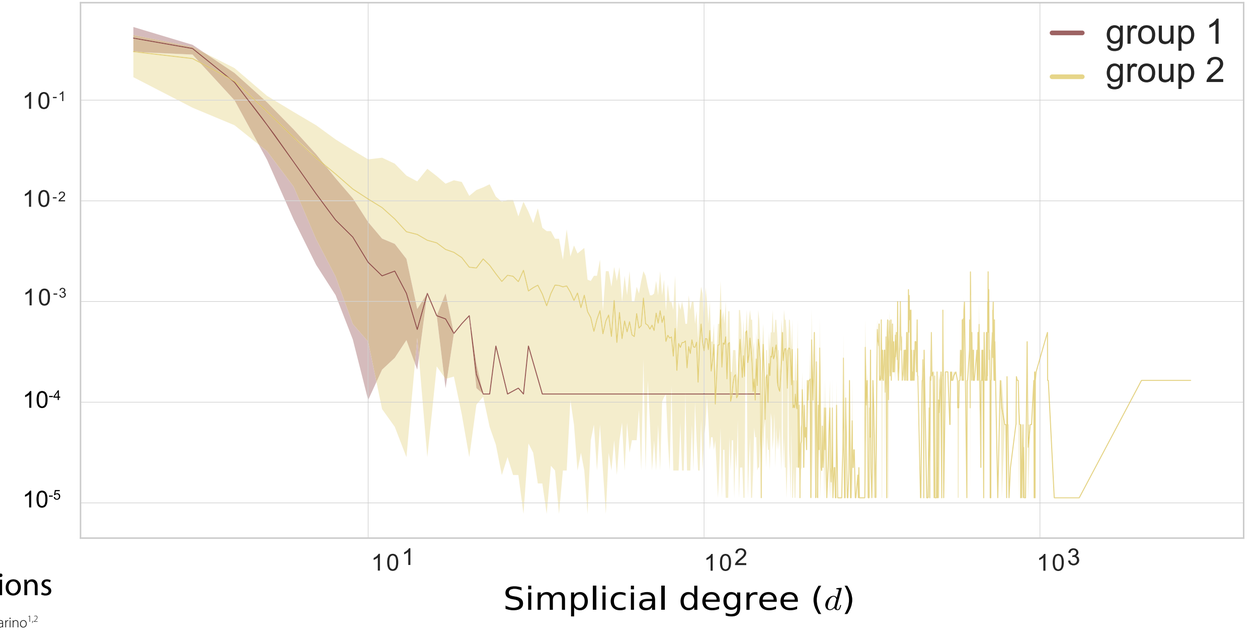

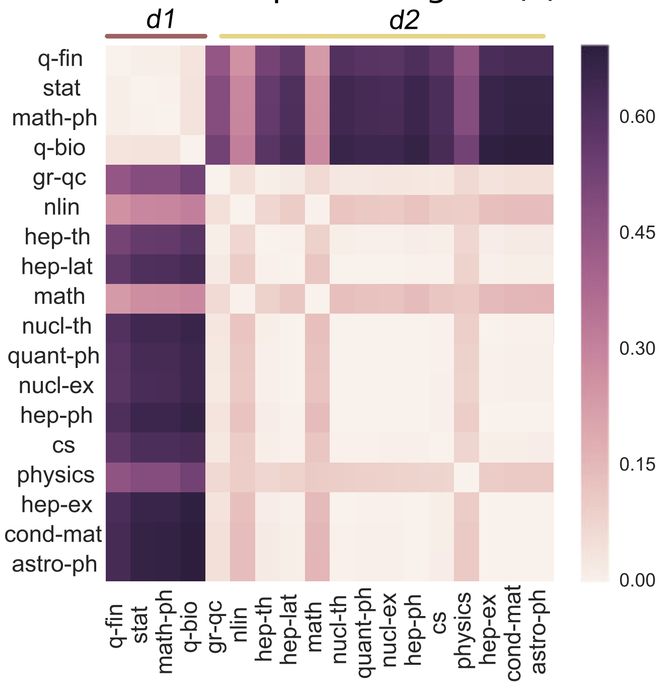

The shape of collaborations

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Do high-order interactions predict new interactions?

- coauth-DBLP
- coauth-MAG-geology
- coauth-MAG-history
- congress-bills
- congress-committees
- threads-stack-overflow
- threads-math-sx
- threads-ask-ubuntu
- contact-high-school
- contact-primary-school
- tags-stack-overflow
- tags-math-sx
- tags-ask-ubuntu
- email-Eu
- email-Enron
- NDC-substances
- NDC-classes
- DAWN
- music-rap-genius

Simplicial closure and higher-order link prediction

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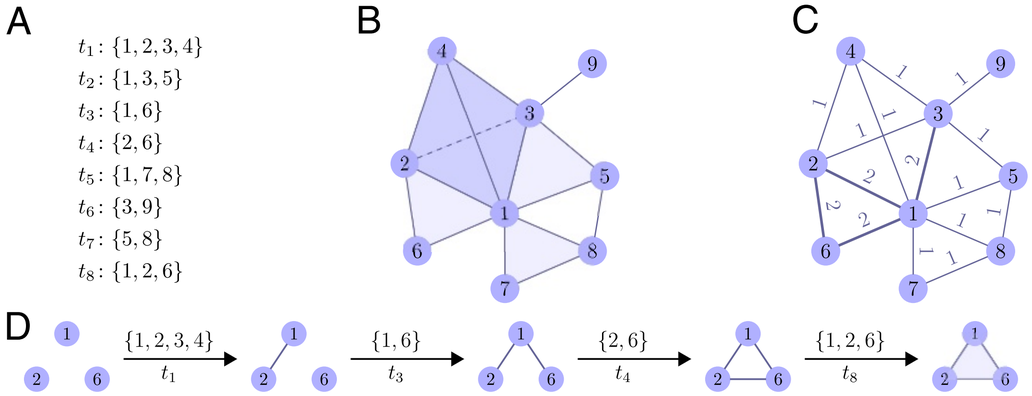

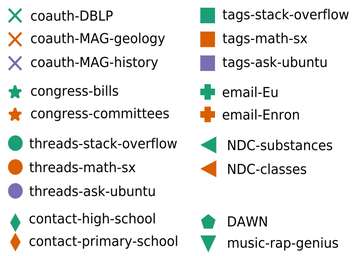

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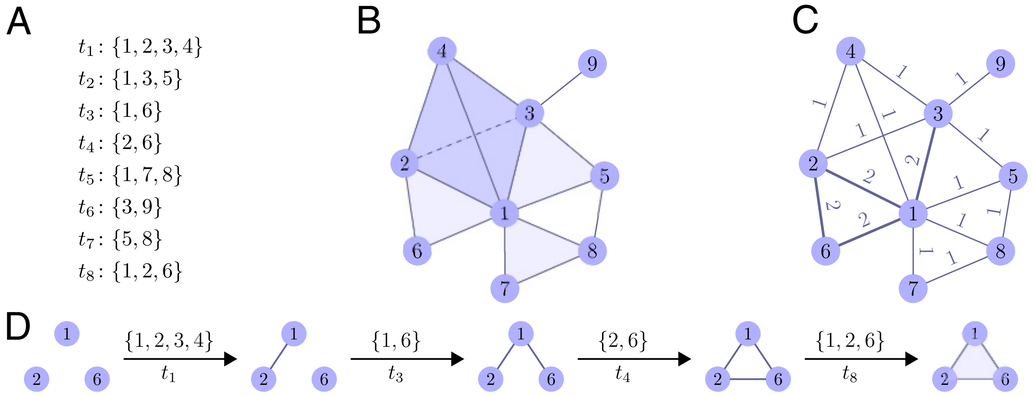

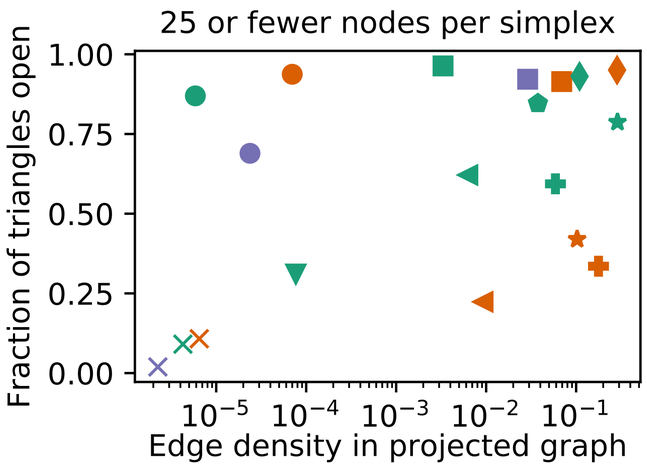

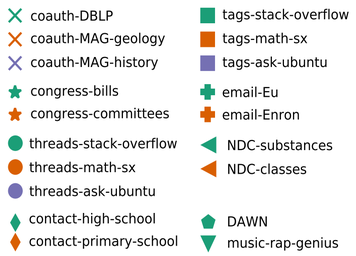

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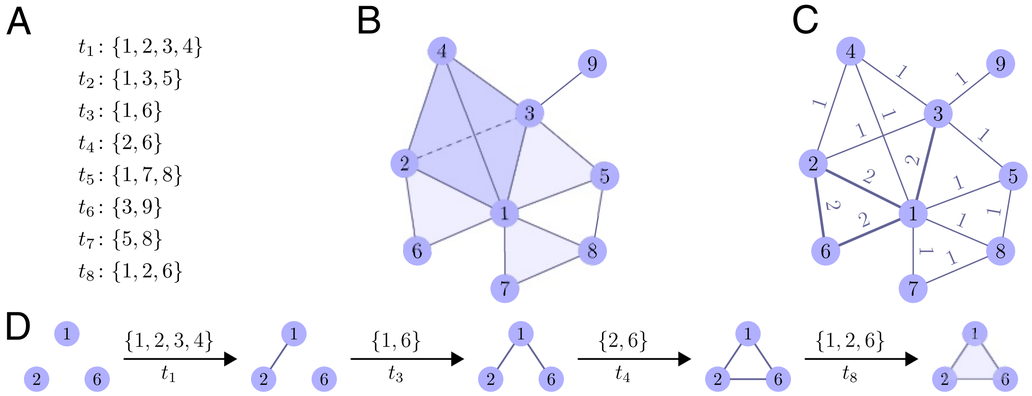

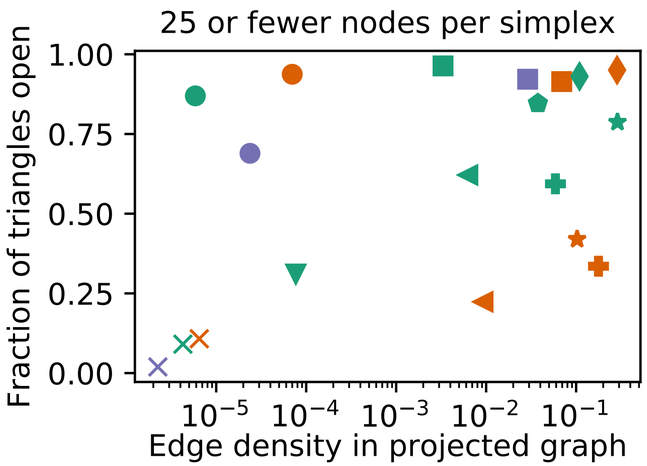

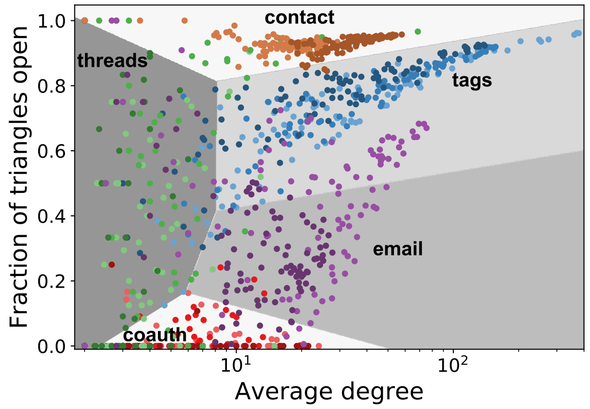

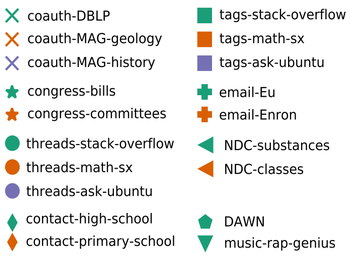

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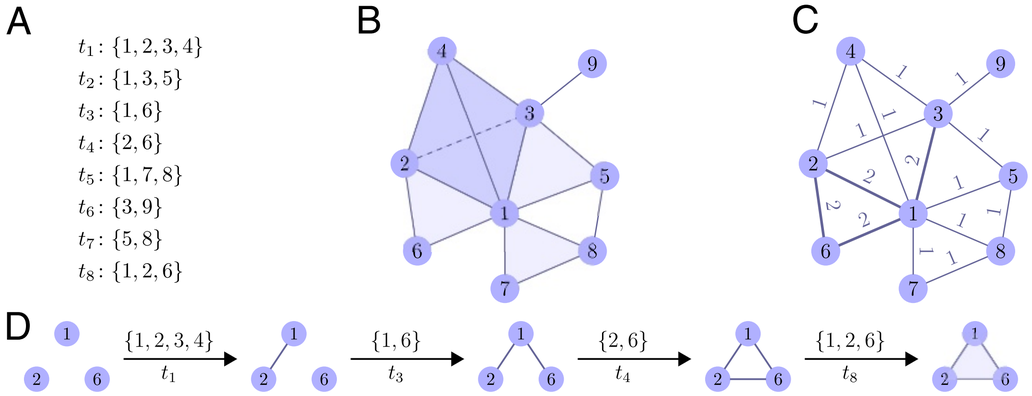
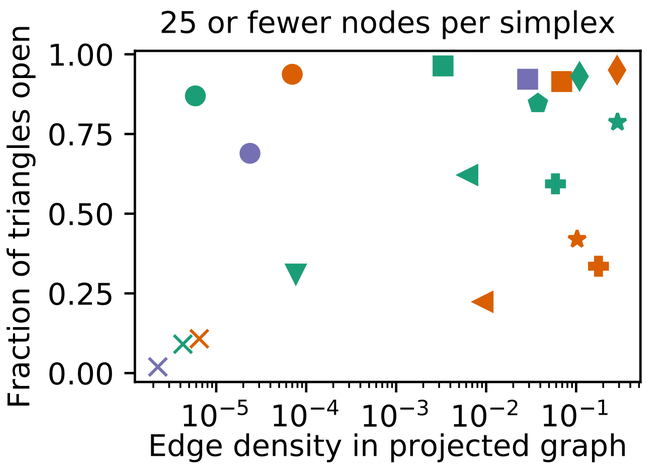
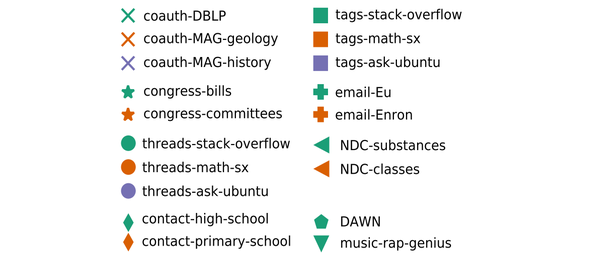
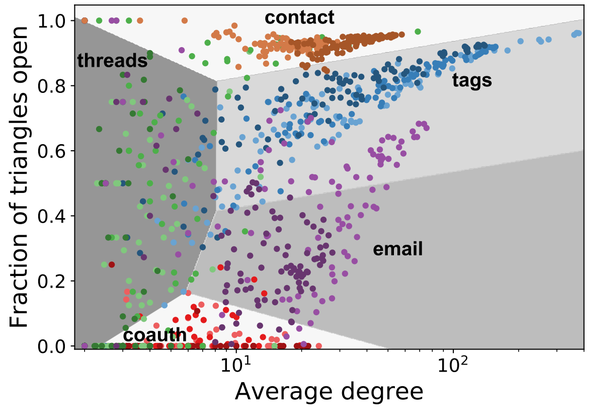
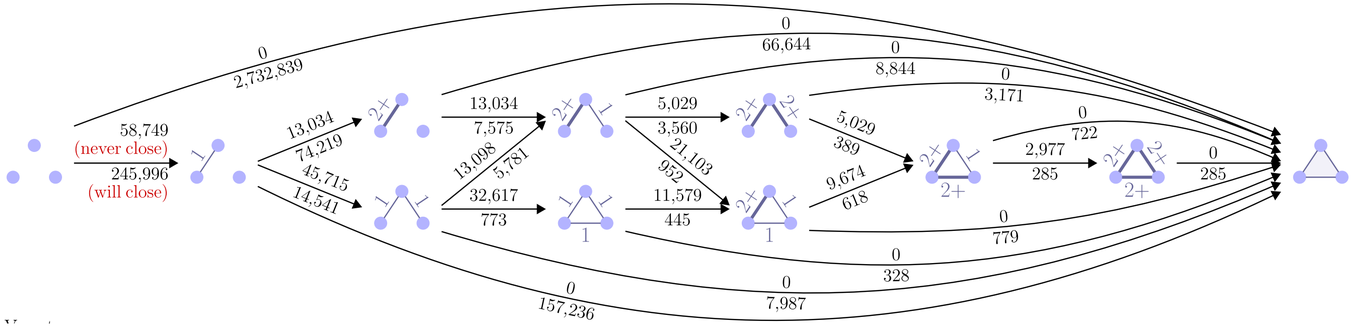








Closure paths



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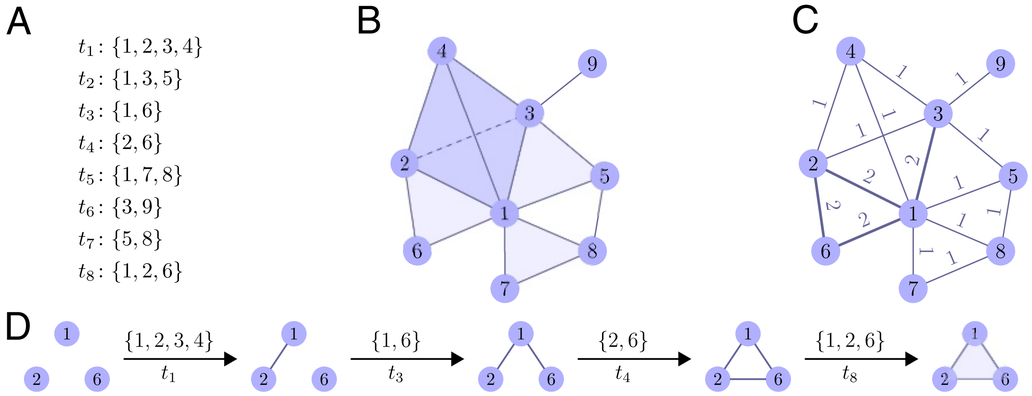

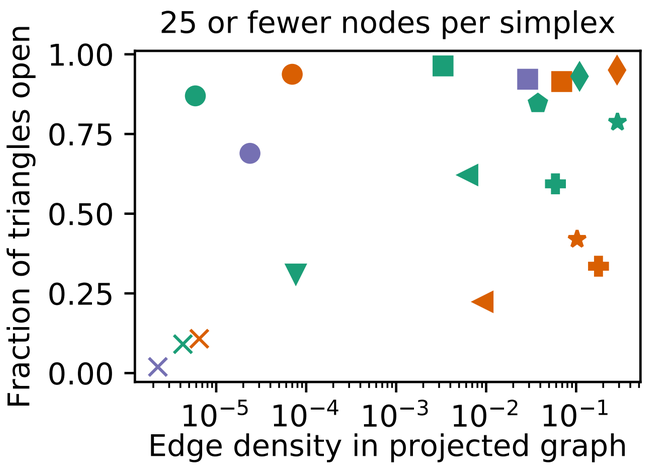

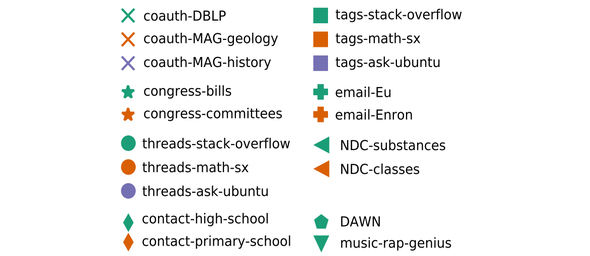

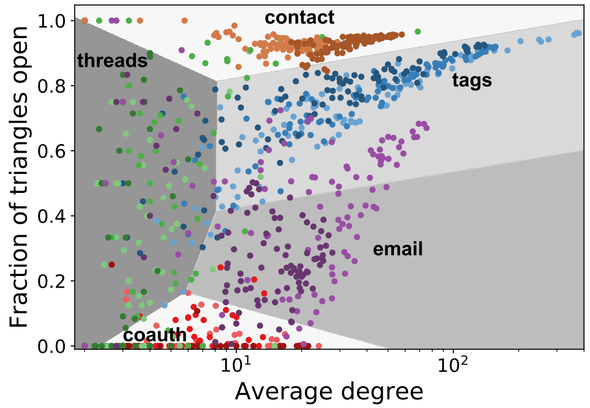

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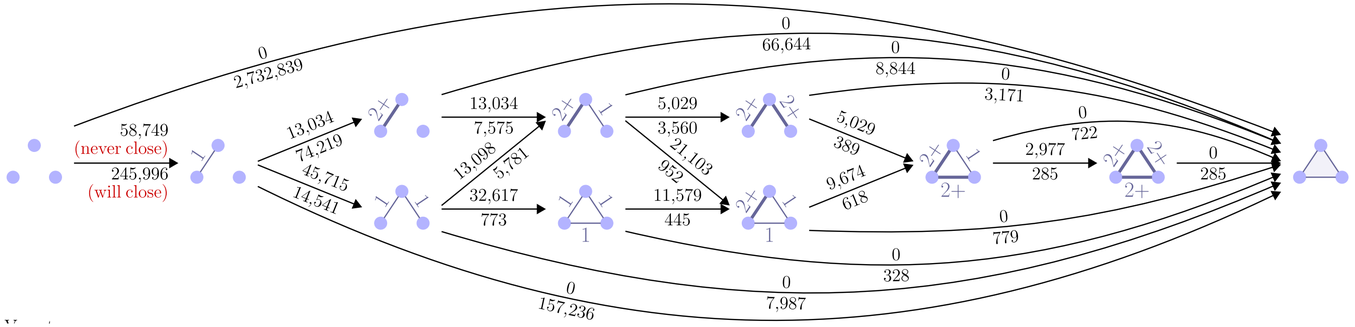

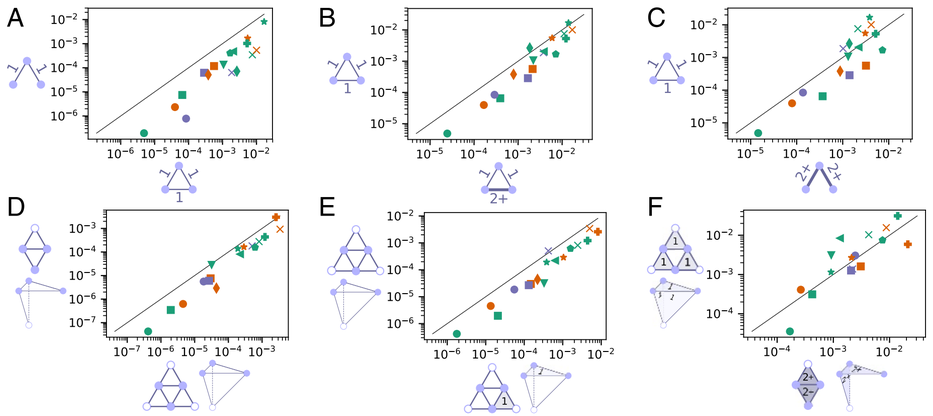

Closure probabilities

Simplicial closure and higher-order link prediction

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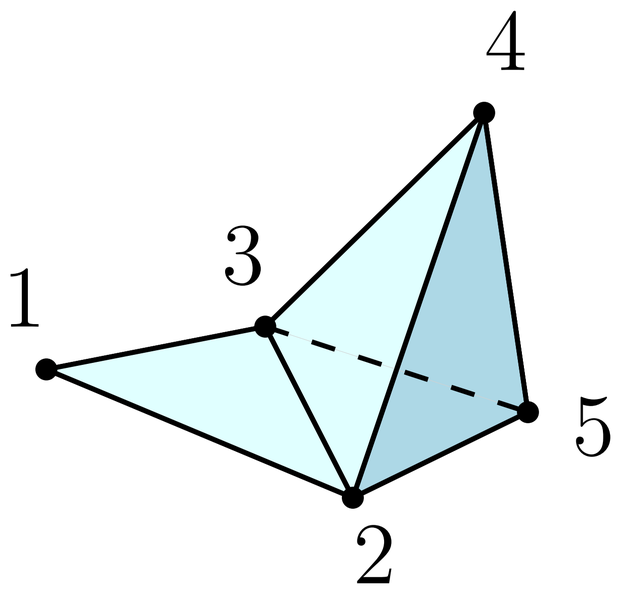
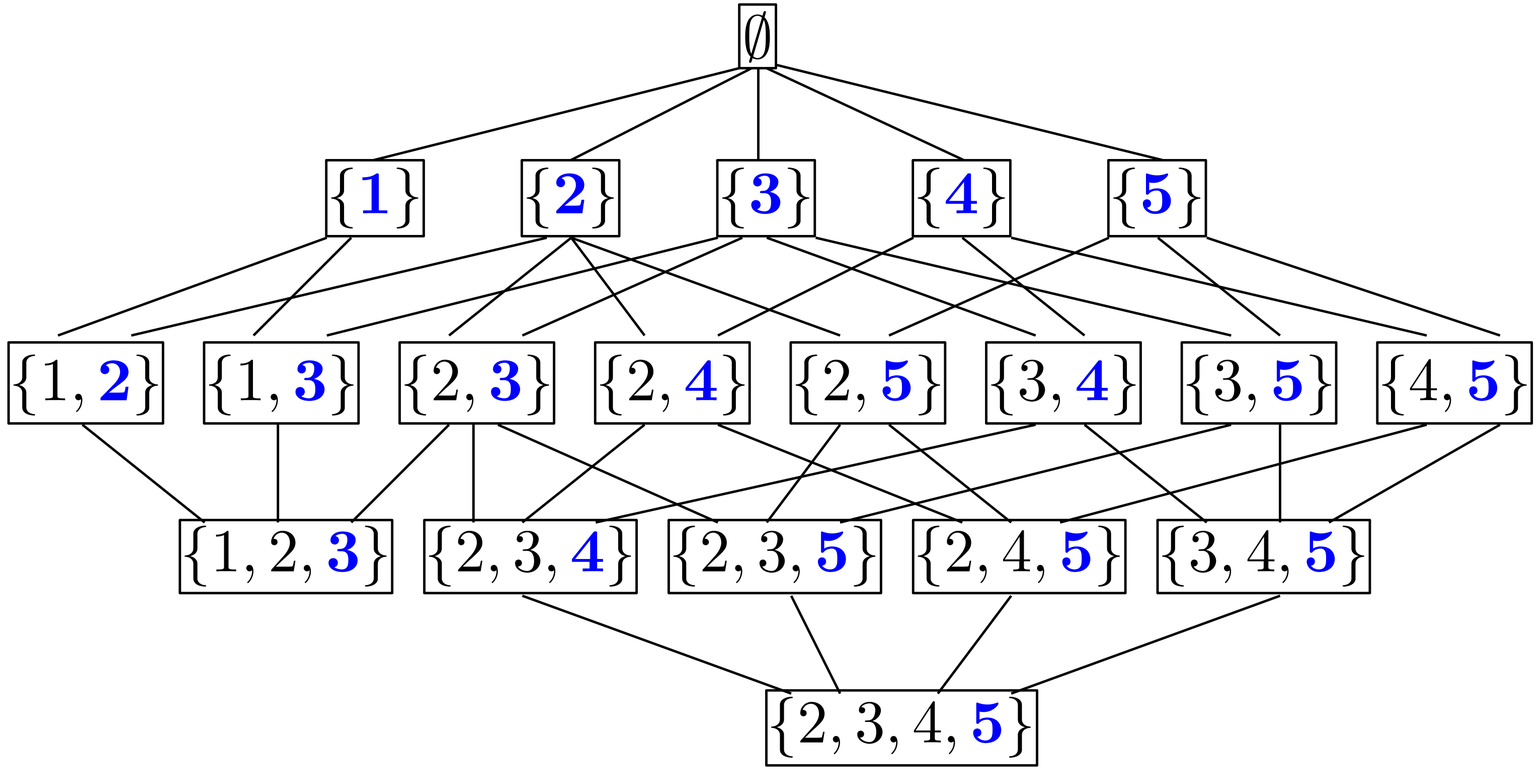
Back to basics: Hasse diagram





Cl´ement Maria. Algorithms and data structures in computational topology. Other. Universit´e Nice Sophia Antipolis, 2014..

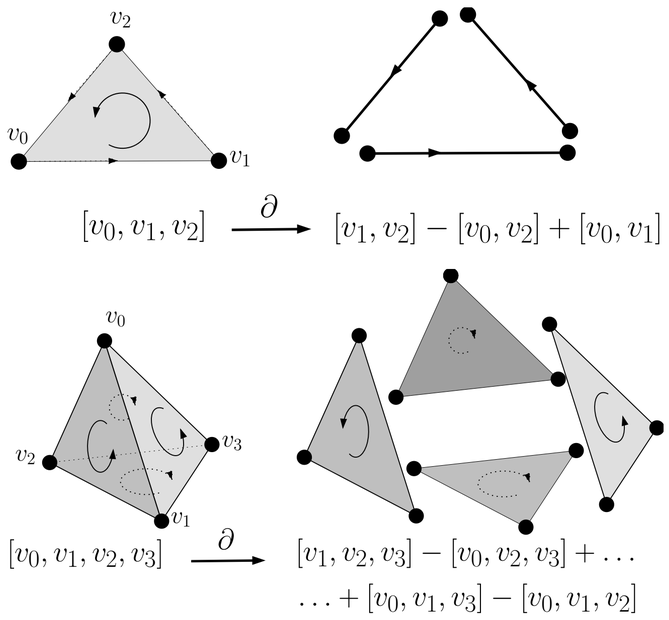
Back to basics: Homology

C_n the k-vector space with basis n-dimensional faces of X and

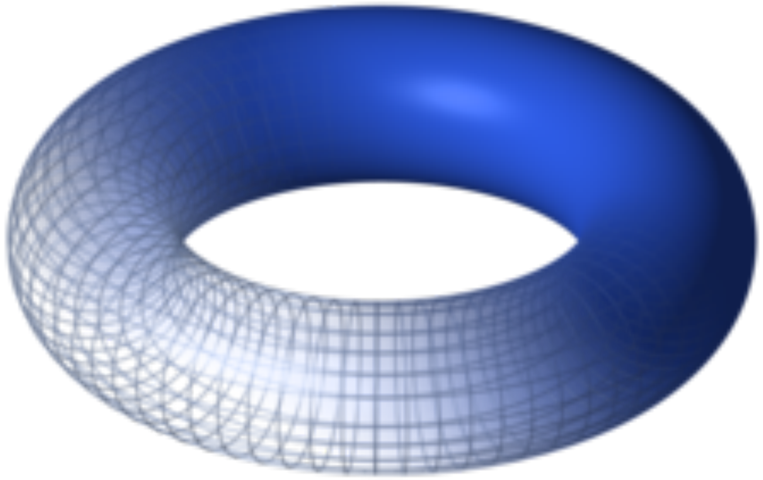
$\partial_n : \quad C_n \to C_{n-1}$ the boundary operator

$$\partial_n[p_1, \ldots, p_n] = \sum_{i=1}^{n} (-1)^i [p_1, \ldots, \hat{p}_i, \ldots, p_n]$$

fit in $\quad C(X) : 0 \to C_t \to \ldots \to C_n \to \ldots C_0 \to 0$



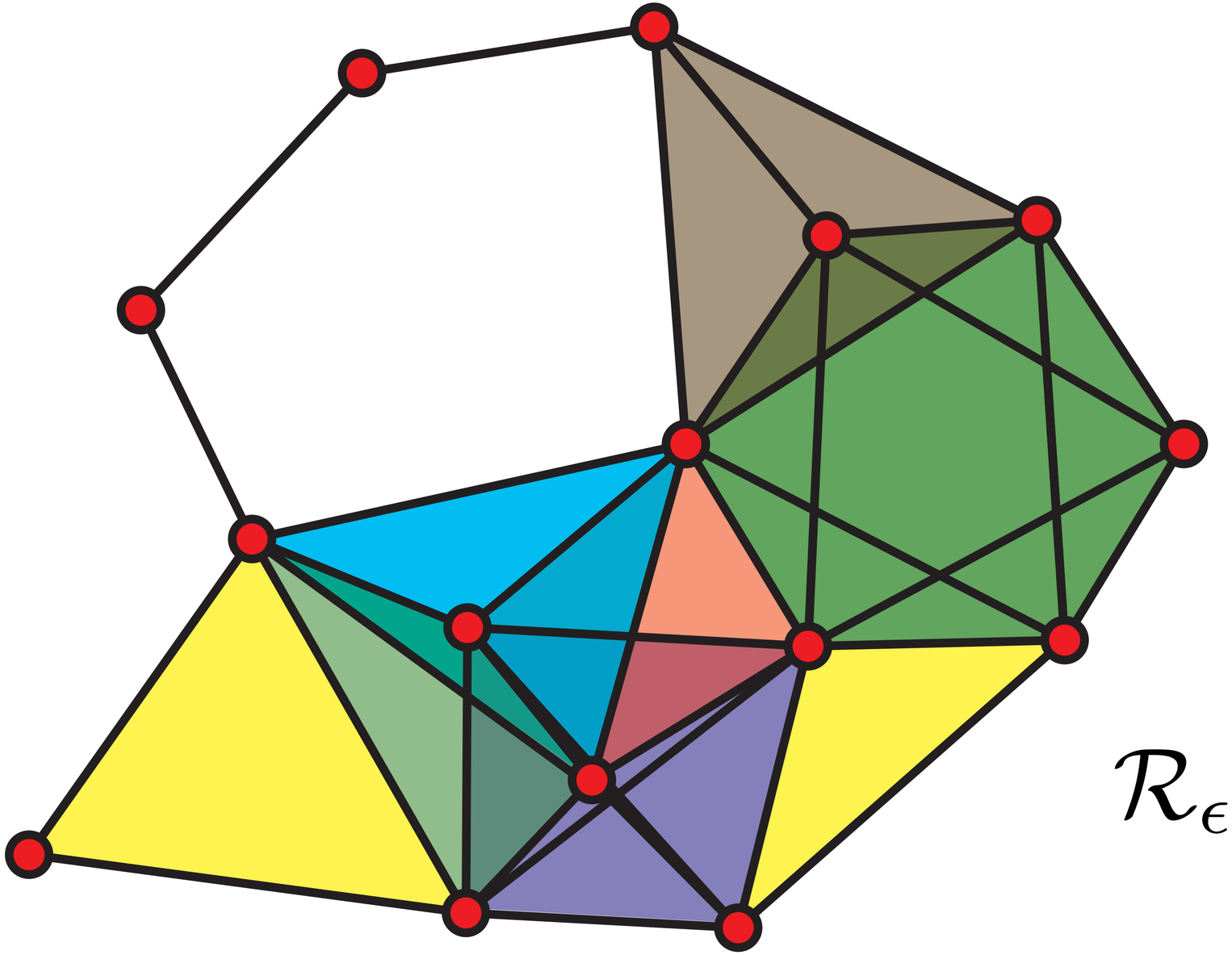
and finally $\quad H_n = \dfrac{\ker \partial_n}{\mathrm{Im} \partial_{n+1}}$

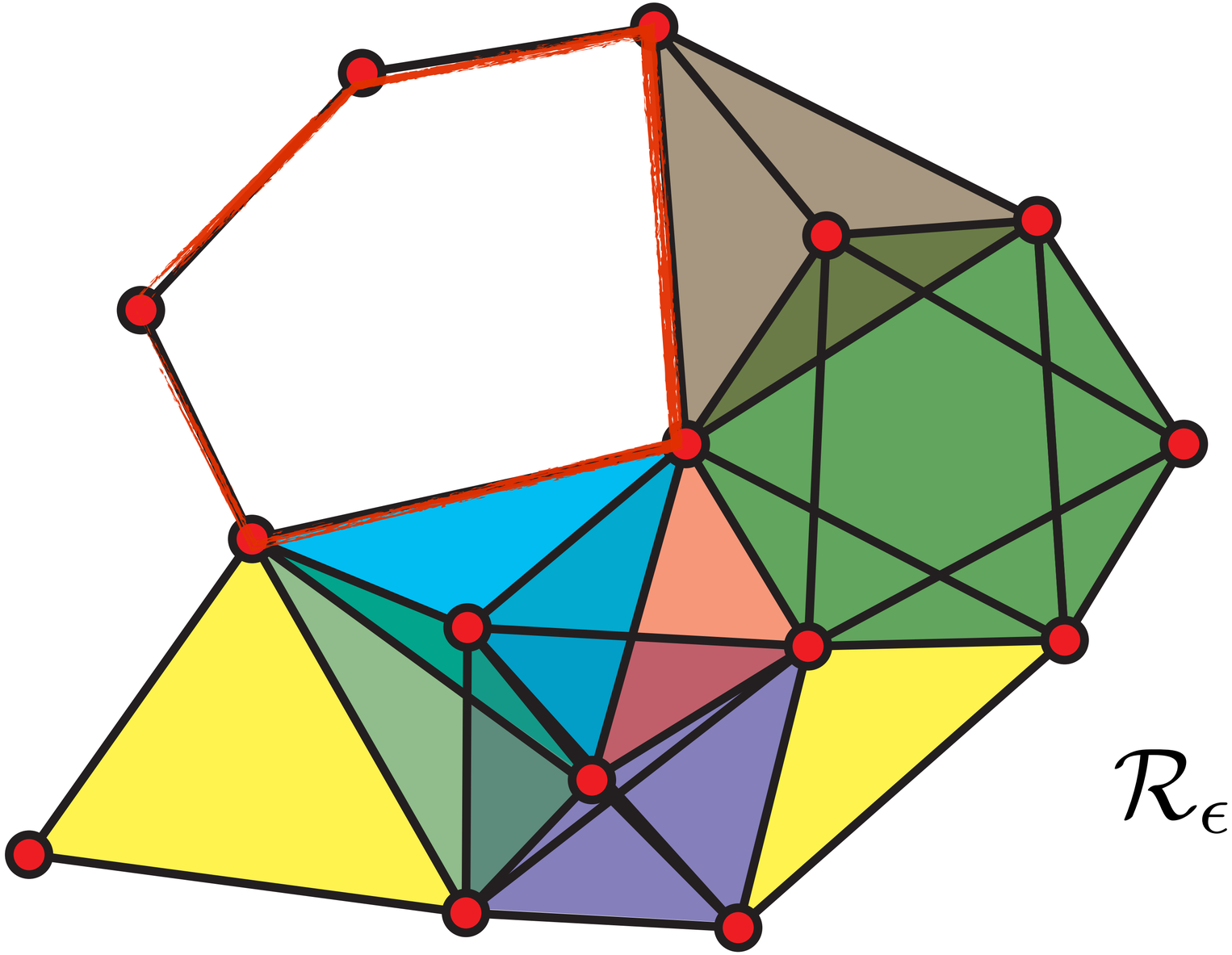


H_0 Conn. components (1)

H_1 Holes (2)

H_2 Voids (1)


$\mathcal{R}_\epsilon$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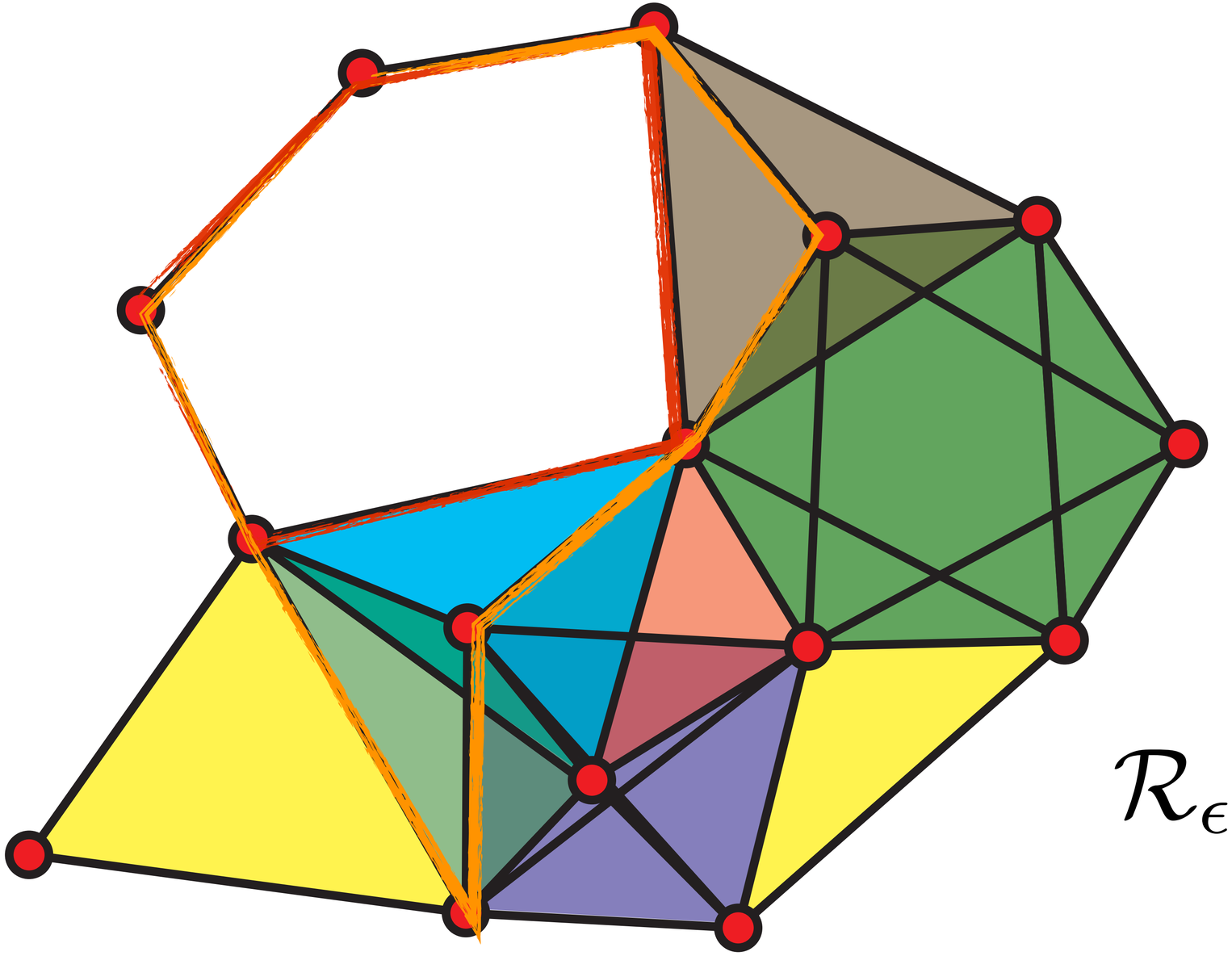
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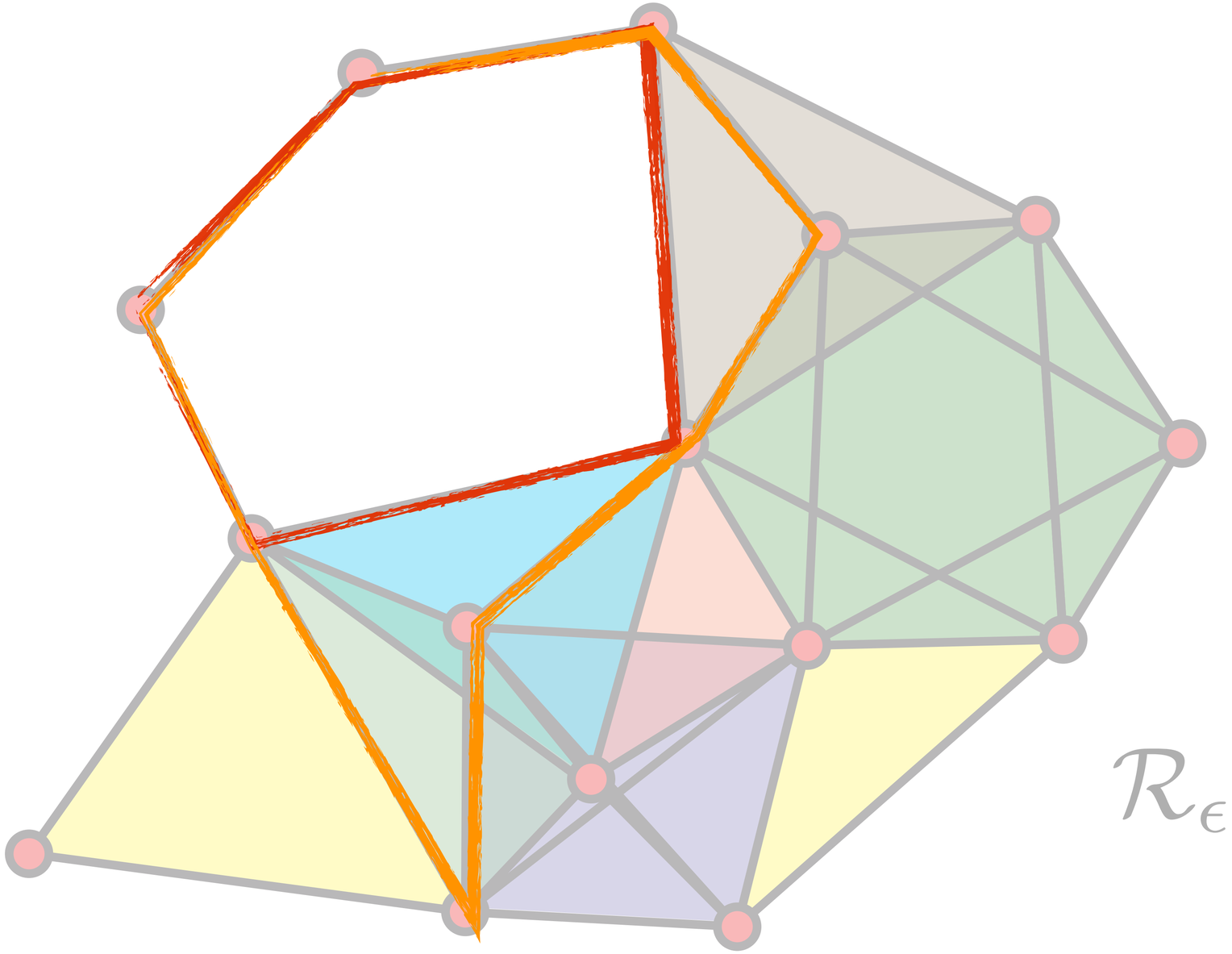
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Back to basics: ....

Control Using Higher Order Laplacians in Network Topologies

Abubakr Muhammad and Magnus Egerstedt

Solid and Physical Modeling with Chain Complexes

Di Carlo et al…

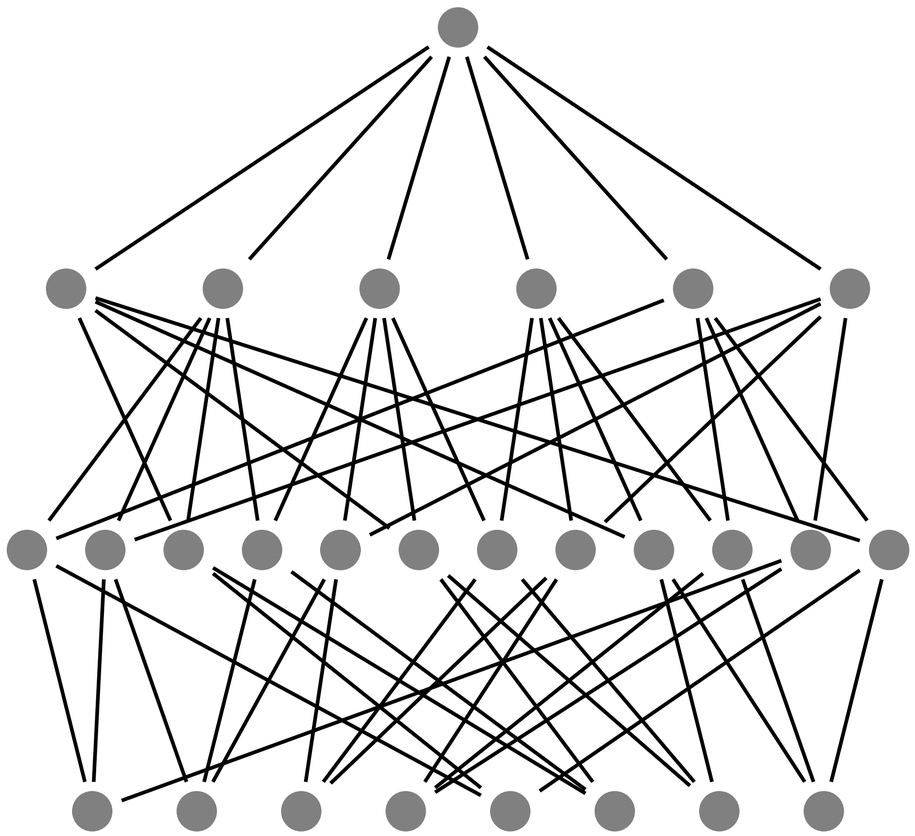
$$\mathcal{H}(K) =$$

$p = 3$

$p = 2$

$p = 1$

$p = 0$



∂_3 δ_2

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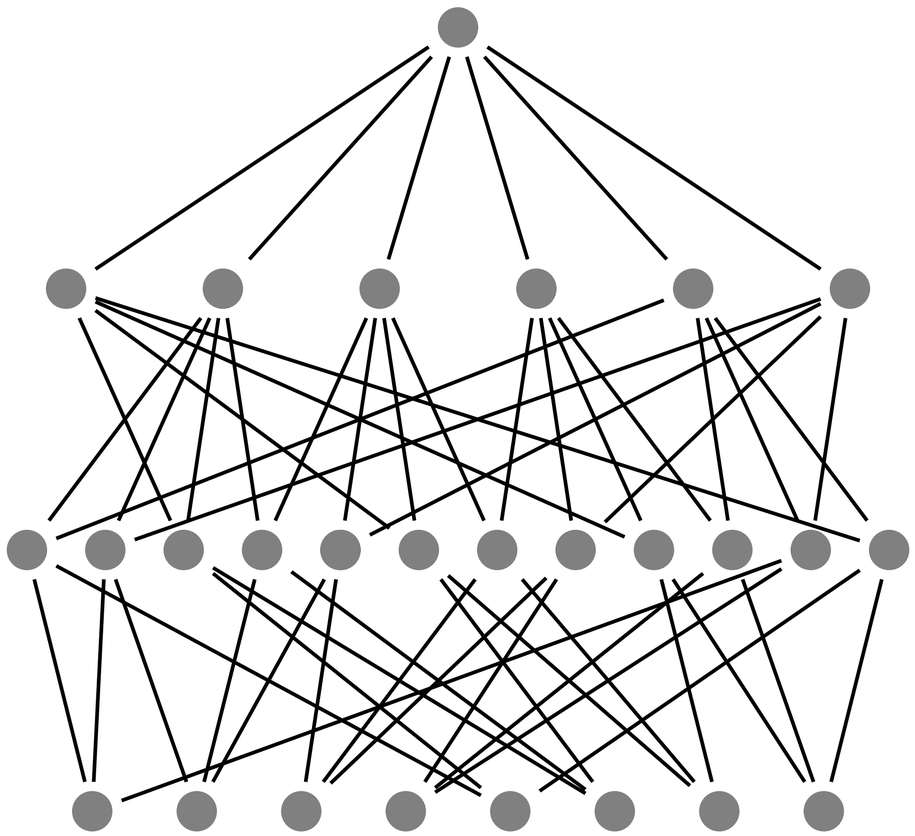

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What is an operator that takes you from k to k?

Back to basics: ....

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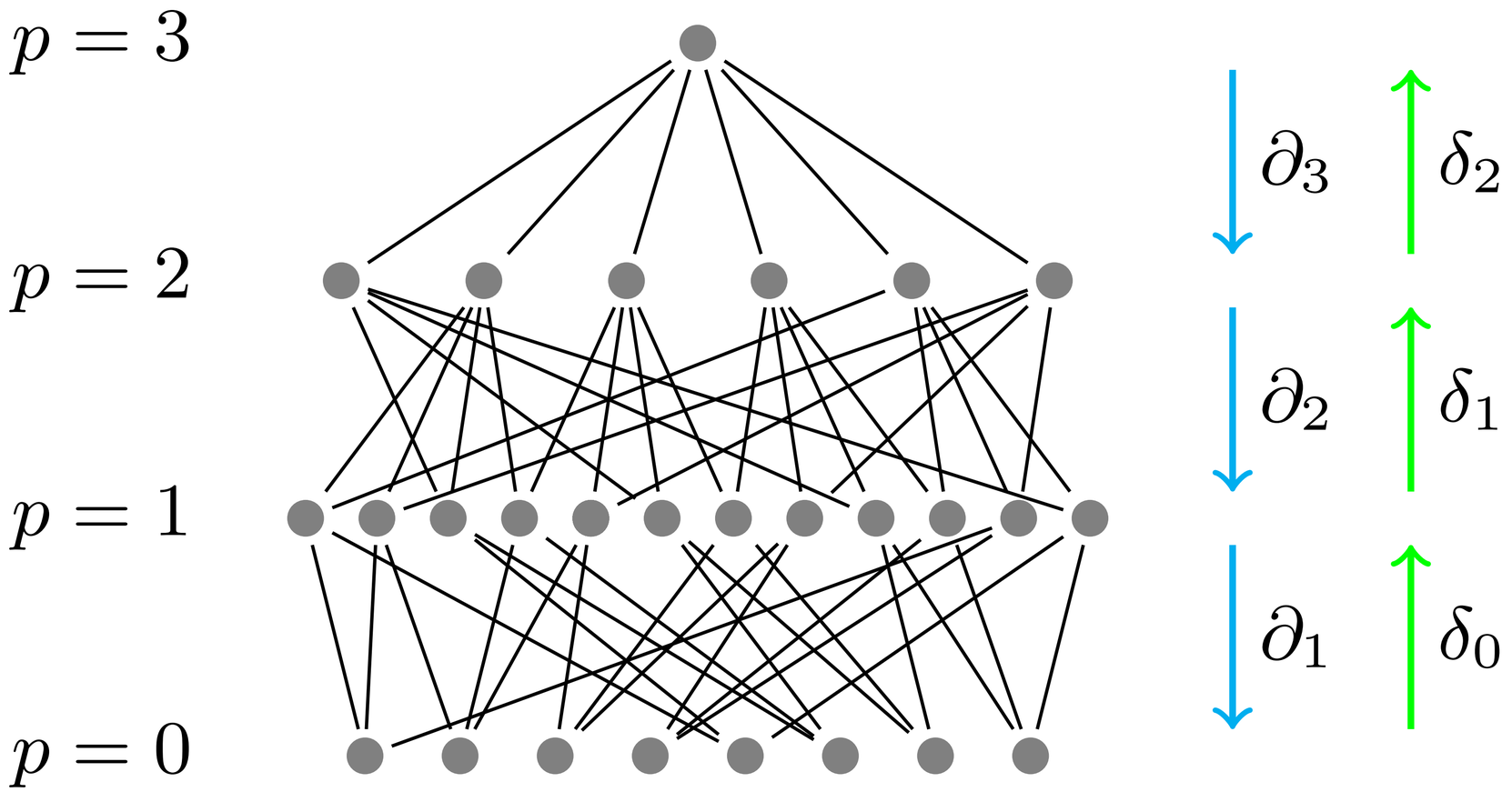

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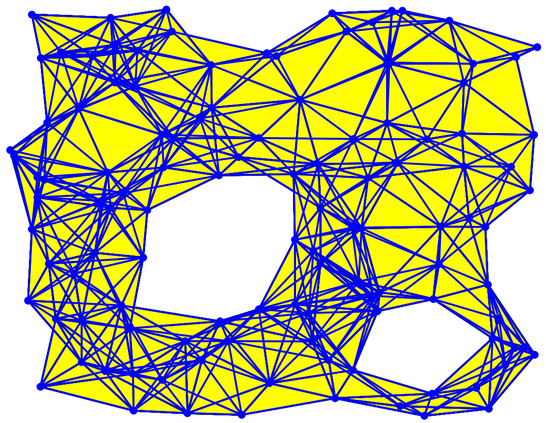

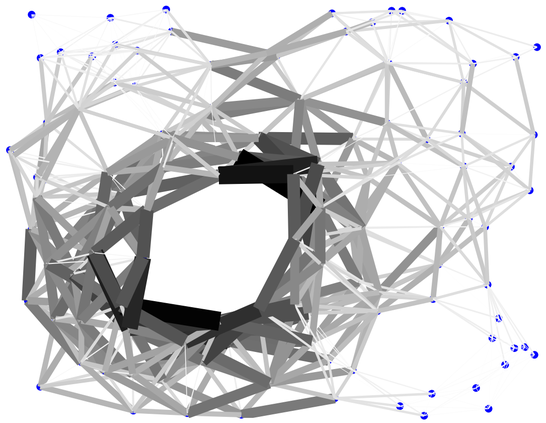

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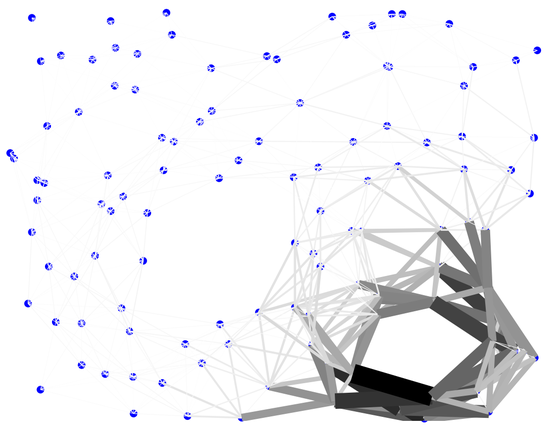

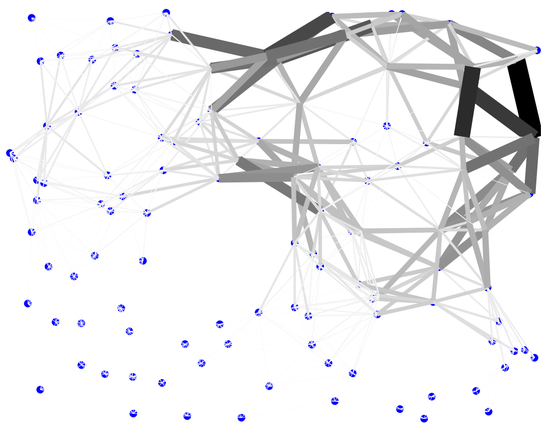

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What happens to dynamics on complexes?

Simplicial PageRank

Based on the k-Laplacian properties

Schaub, Michael T., et al. "Random Walks on Simplicial Complexes and the normalized Hodge Laplacian." *arXiv preprint arXiv:1807.05044* (2018).

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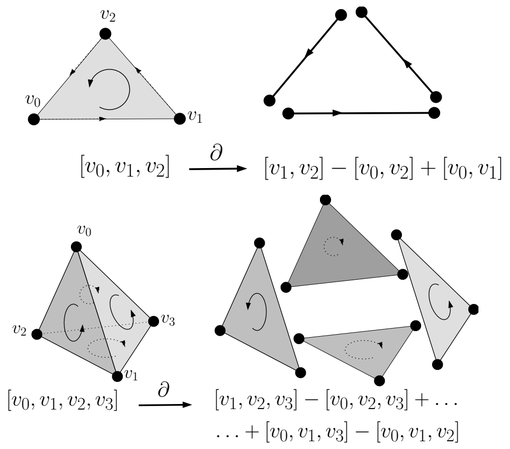

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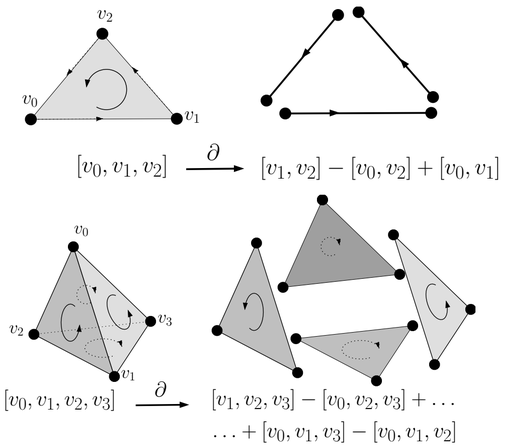

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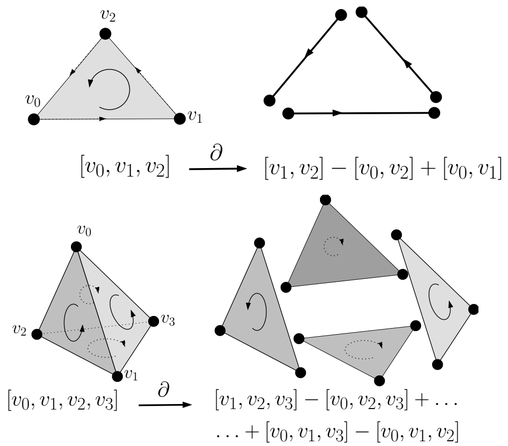

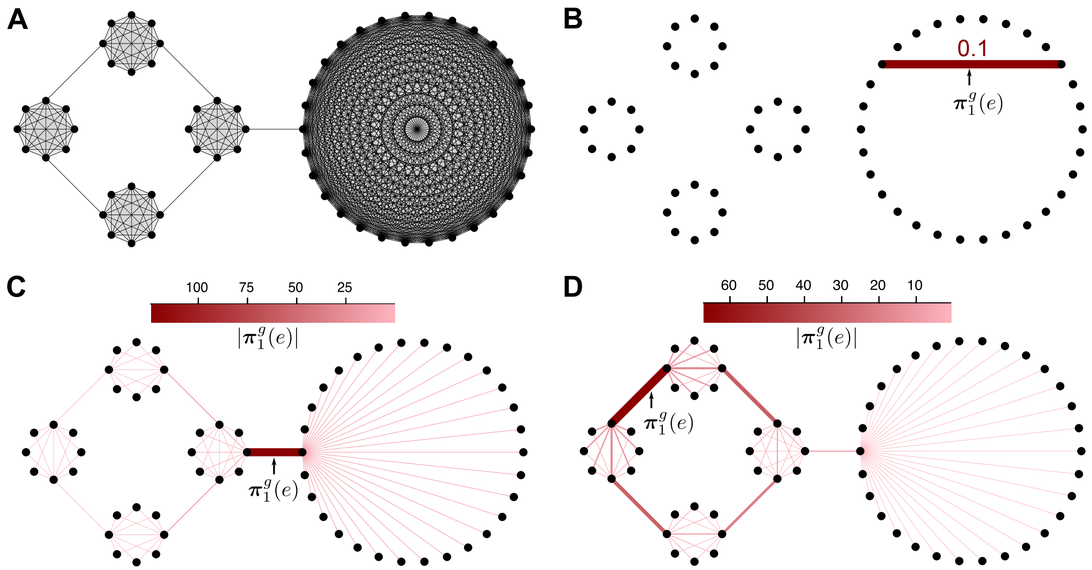

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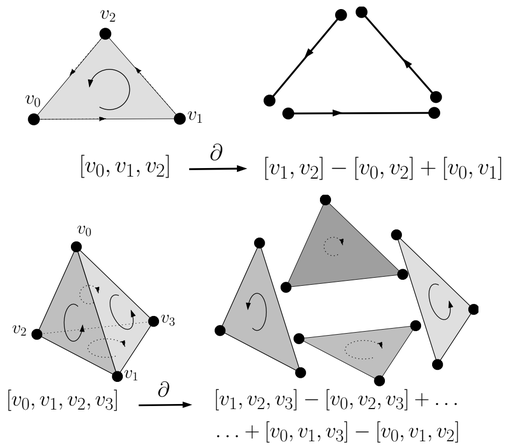
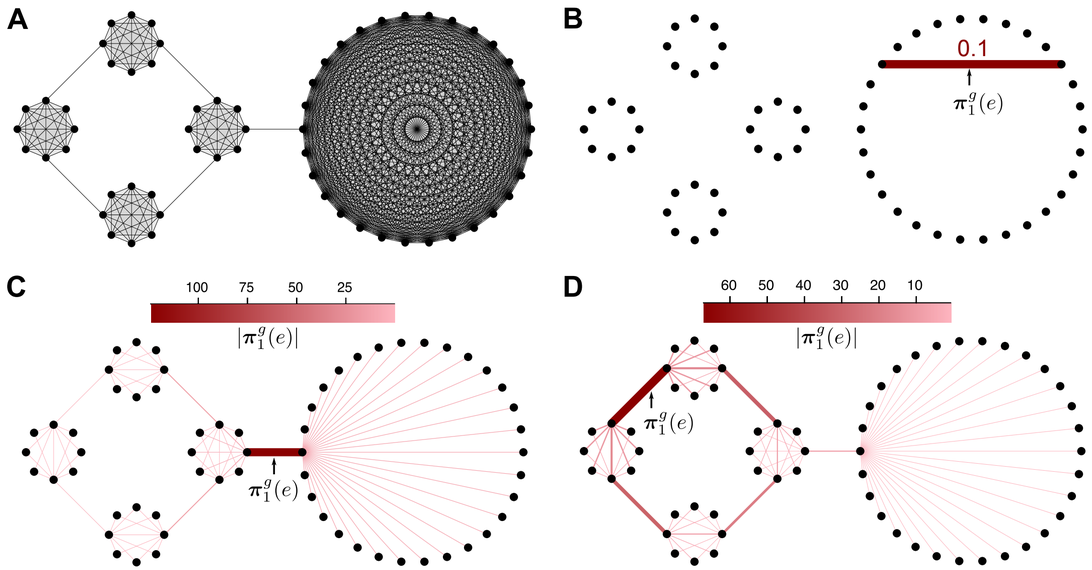
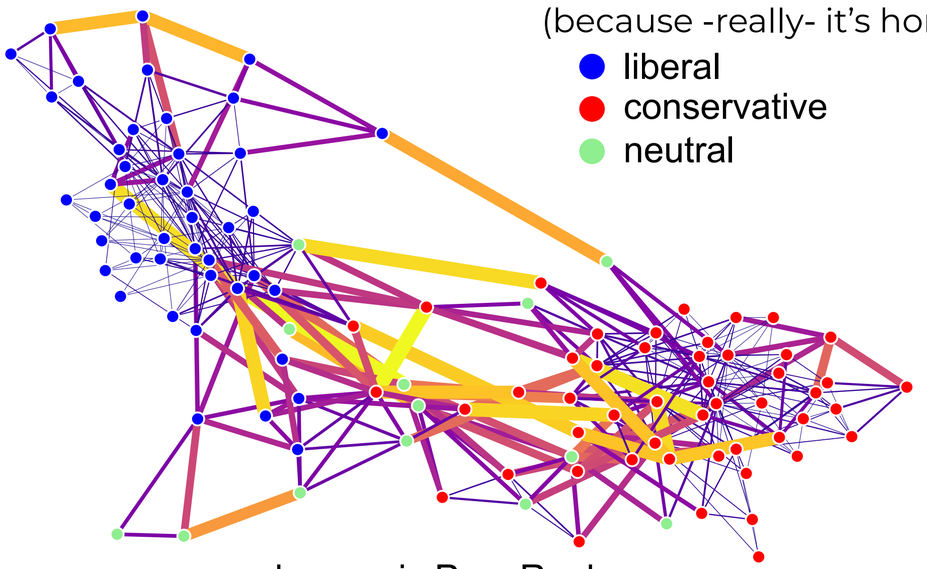




Similar to Patania et al. EPJ Data Science (2017)
(because -really- it's homology!)



harmonic PageRank

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Random null models

Simplest random SC model?

Topology of random simplicial complexes: a survey

Matthew Kahle

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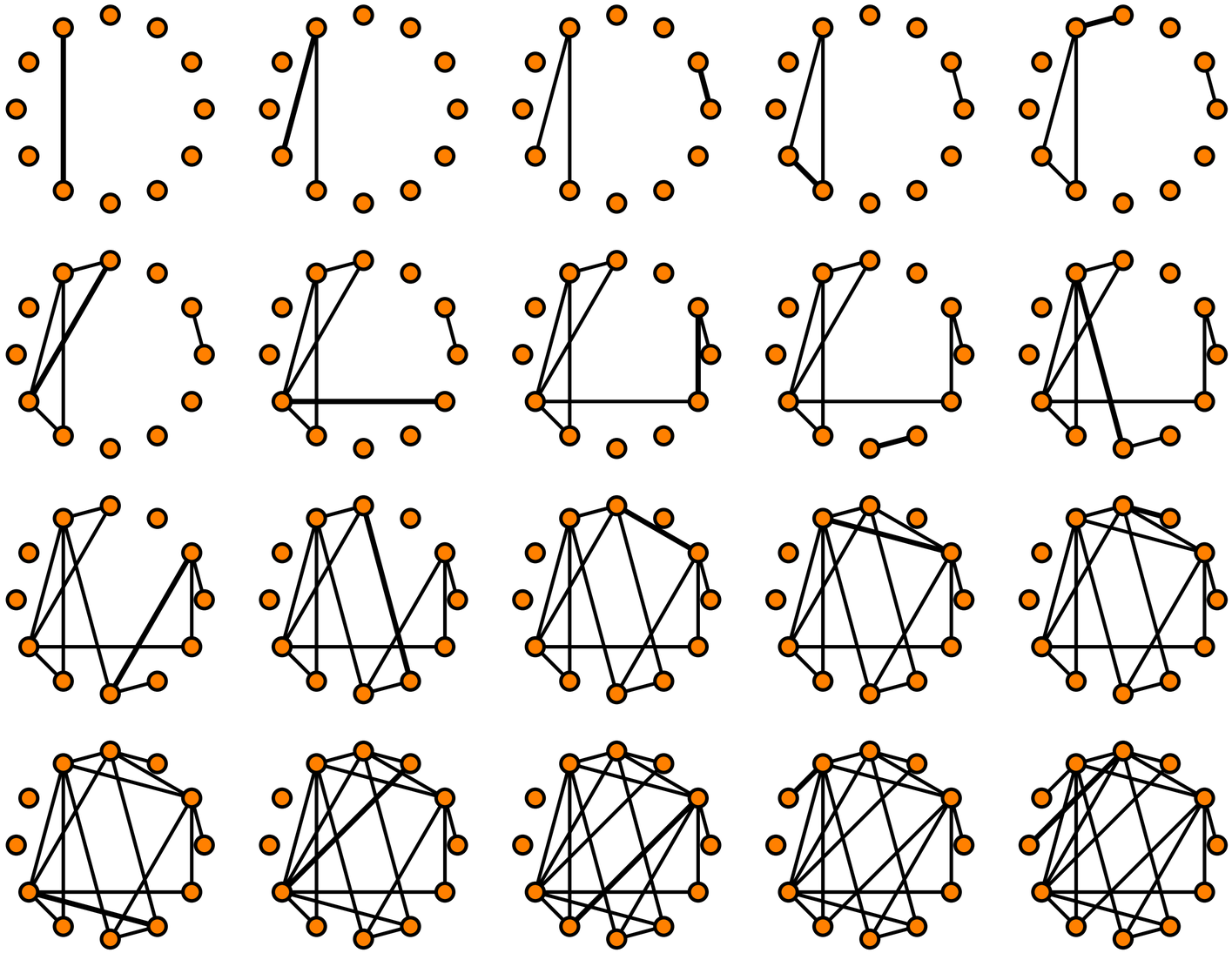

Topology of random simplicial complexes: a survey

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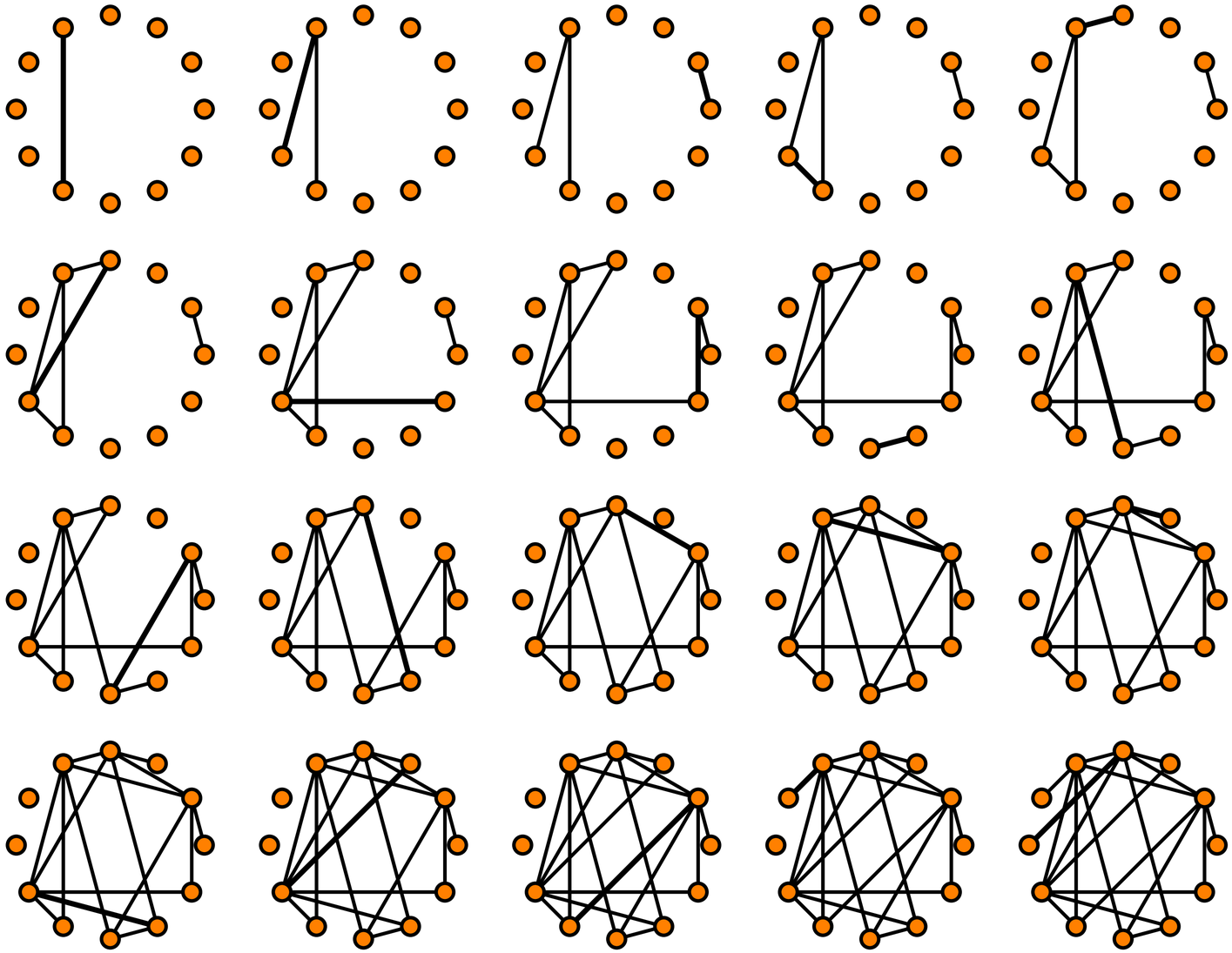

Topology of random simplicial complexes: a survey

Matthew Kahle

THEOREM 2.1 (Erdős–Rényi, 1959). *Let $\epsilon > 0$ be fixed, and $G \sim G(n,p)$. If*

$$p \geq \frac{(1+\epsilon)\log n}{n},$$

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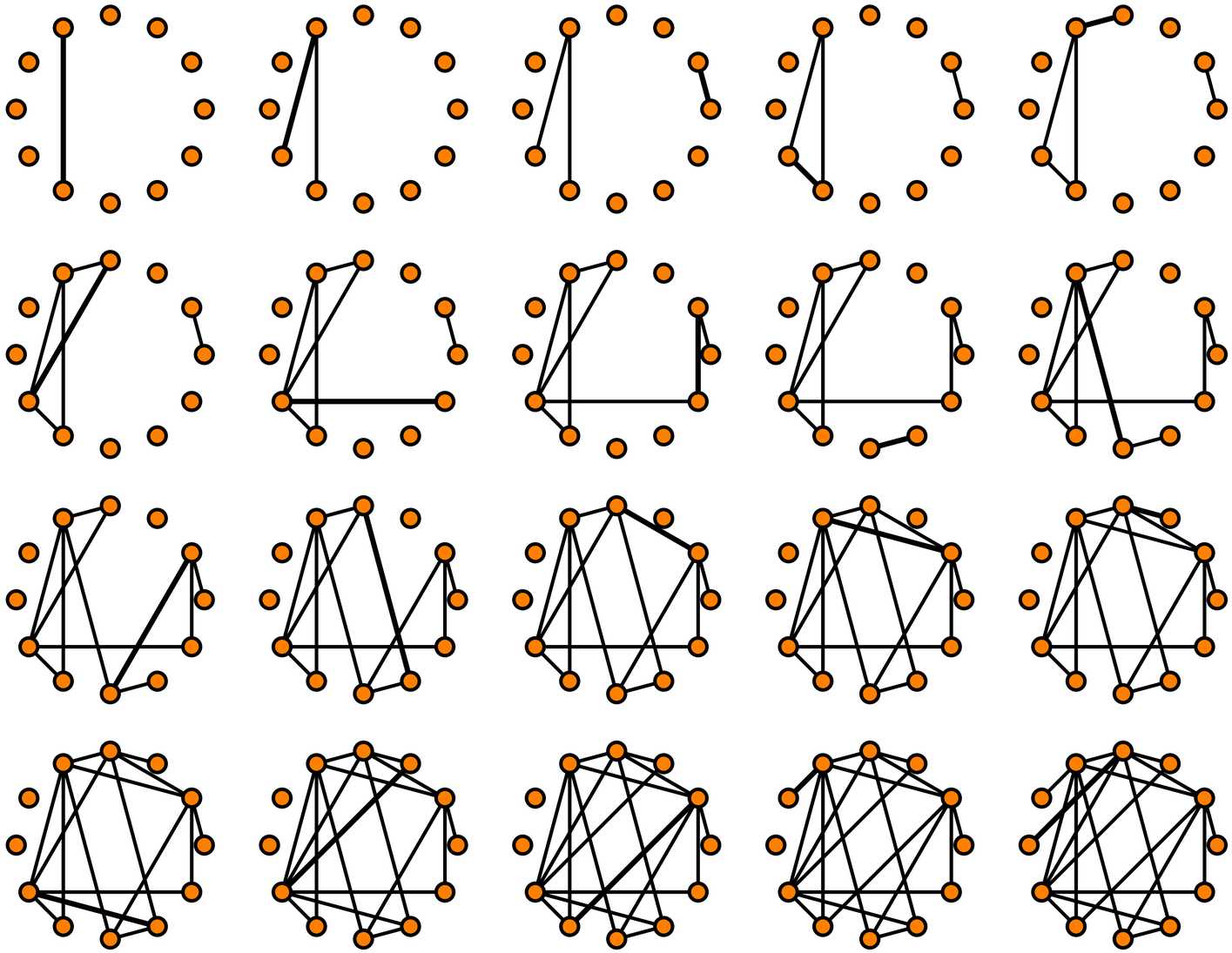

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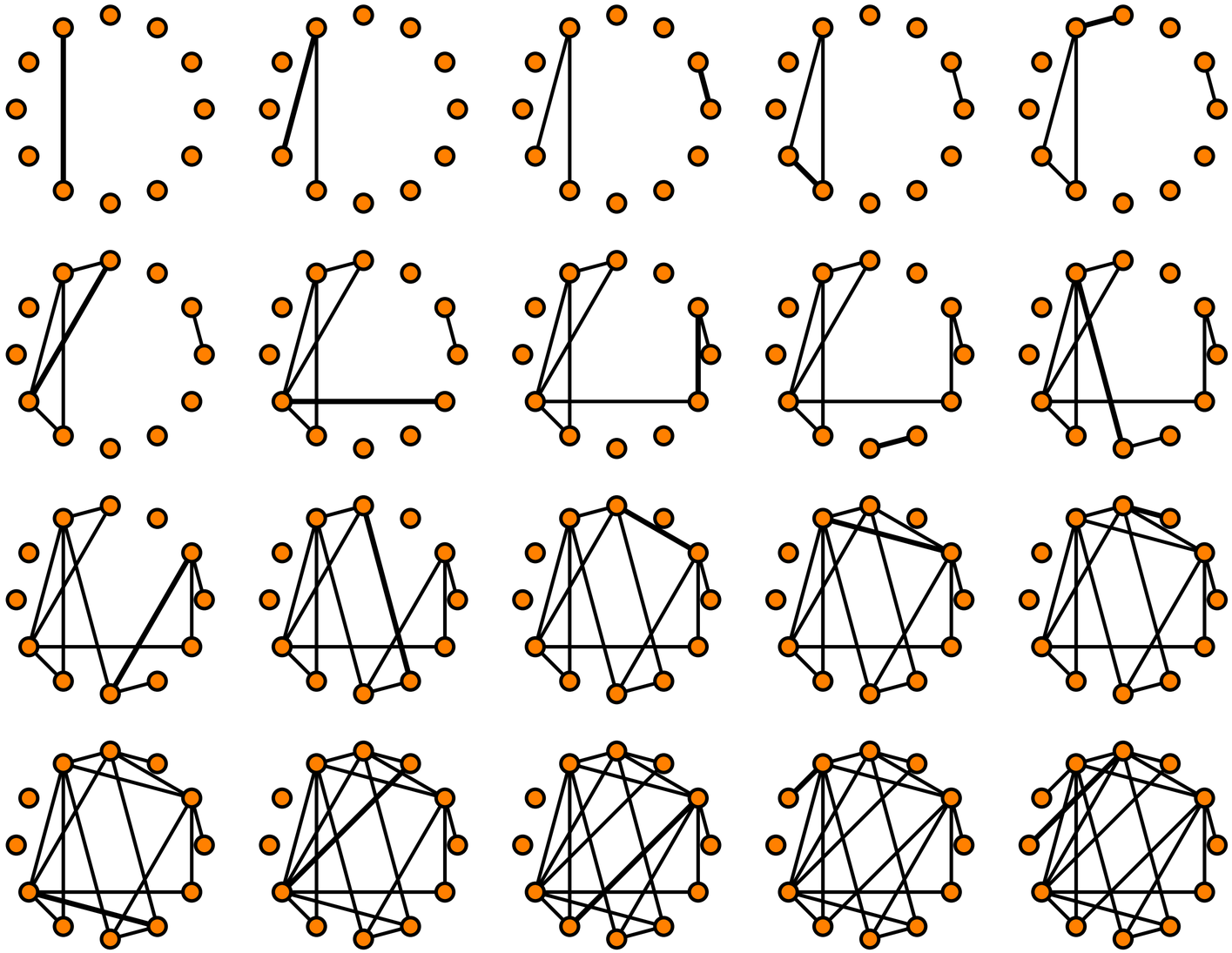

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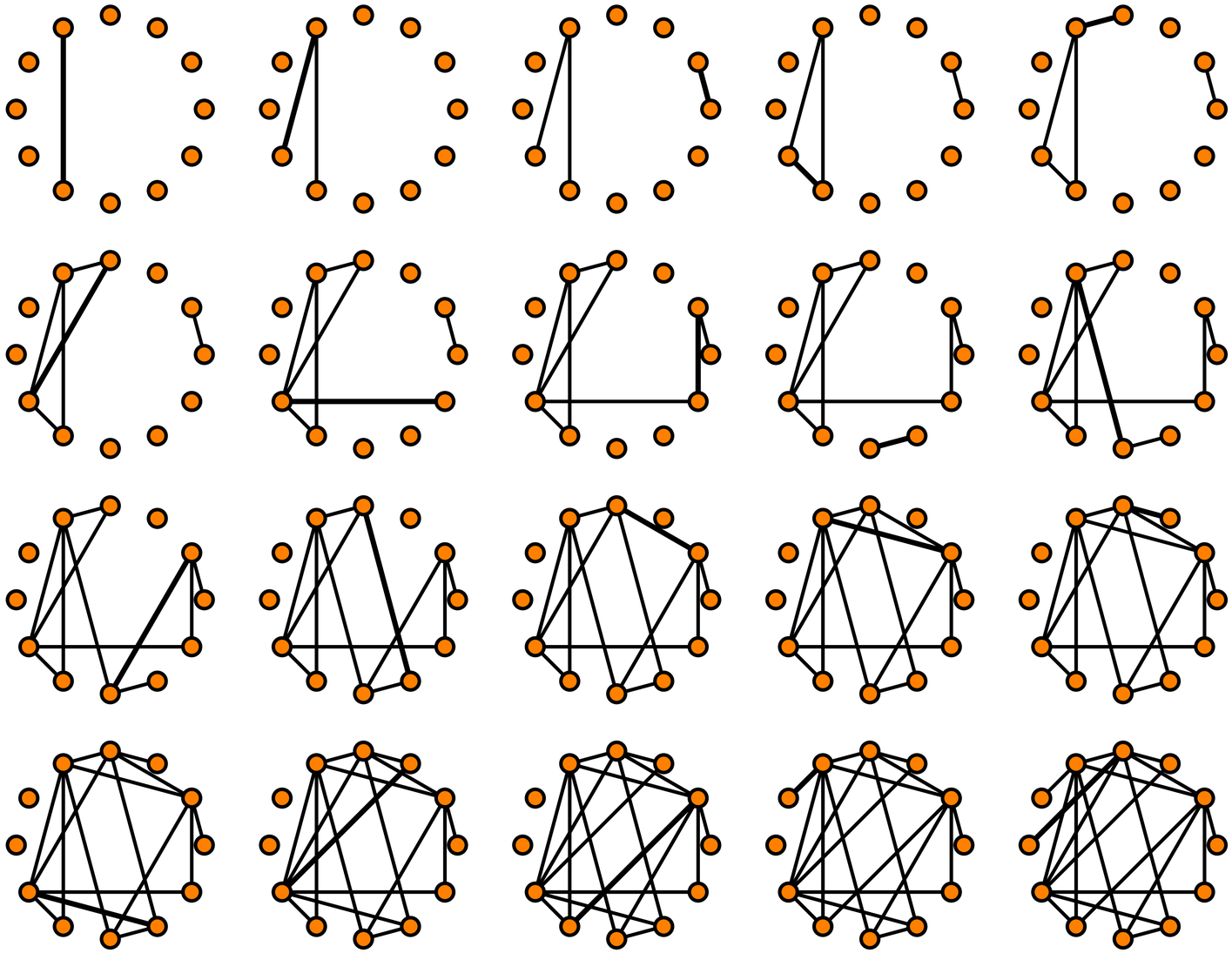

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$$\tilde{\beta}_0 = \#\text{ conn comps} - 1$$

Simplest* random SC model?

THEOREM 3.1 (Linial–Meshulam, 2006). *Let $\epsilon > 0$ be fixed and $Y \sim Y(n,p)$. If*

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then w.h.p. $H^1(Y, \mathbb{Z}/2) = 0$, and if

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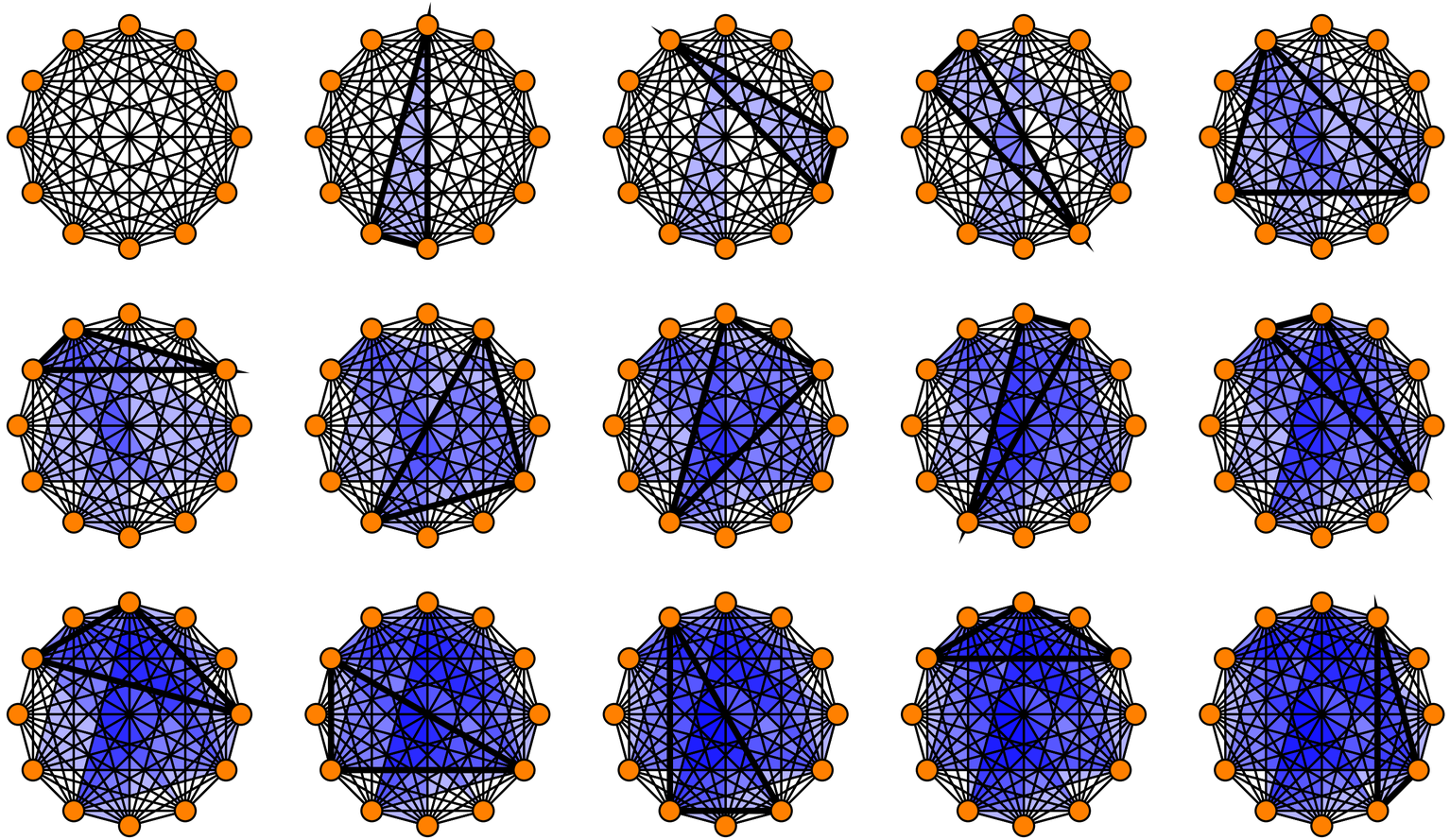
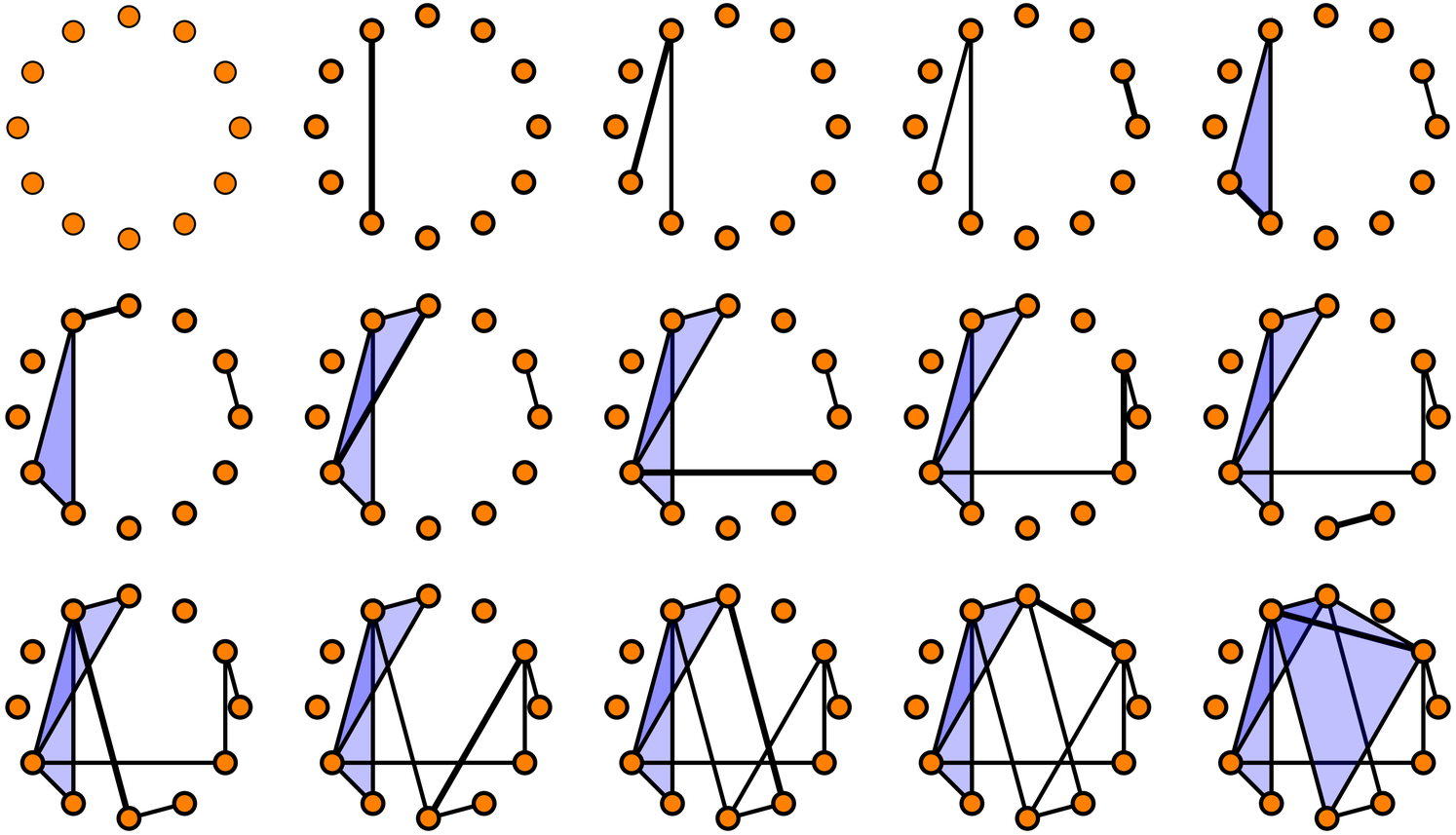
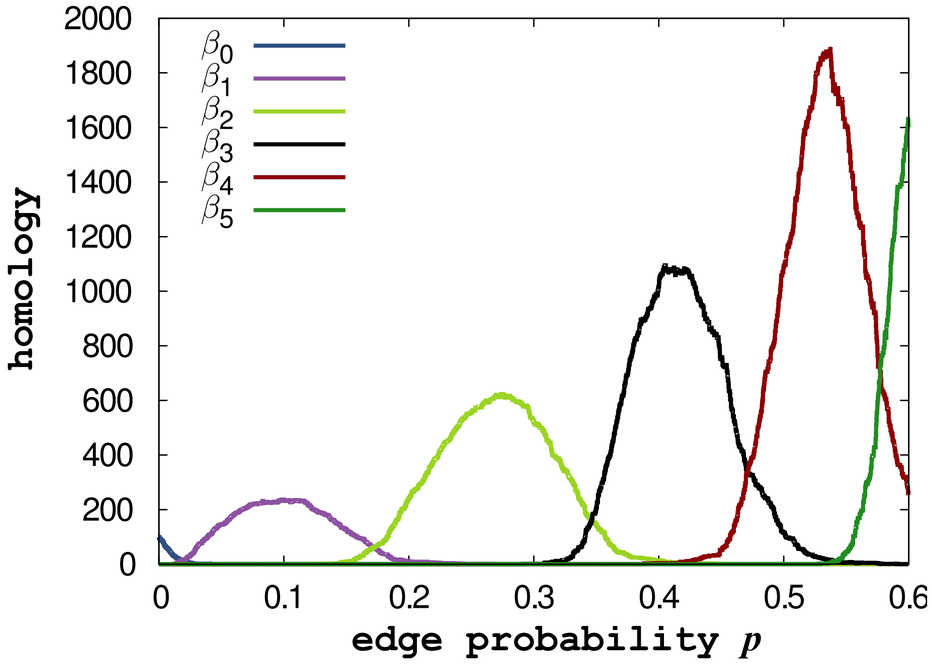


Linial - Meshulam complex

Random Flag complexes

The flag complex $X(H)$ of a graph H is the maximal simplicial complex compatible with H as its 1-skeleton





THEOREM 4.1. *Let $k \geq 1$ and $\alpha > 0$ be fixed, $p = n^{-\alpha}$, and $X \sim X(n,p)$.*

(1) *If $\alpha > 1/k$ then w.h.p. $H_k(X, \mathbb{Z}) = 0$.*

(2) *If $\alpha < 1/(2k+1)$, then w.h.p. $H_k(X, \mathbb{Z}) = 0$.*

Topology of random simplicial complexes: a survey

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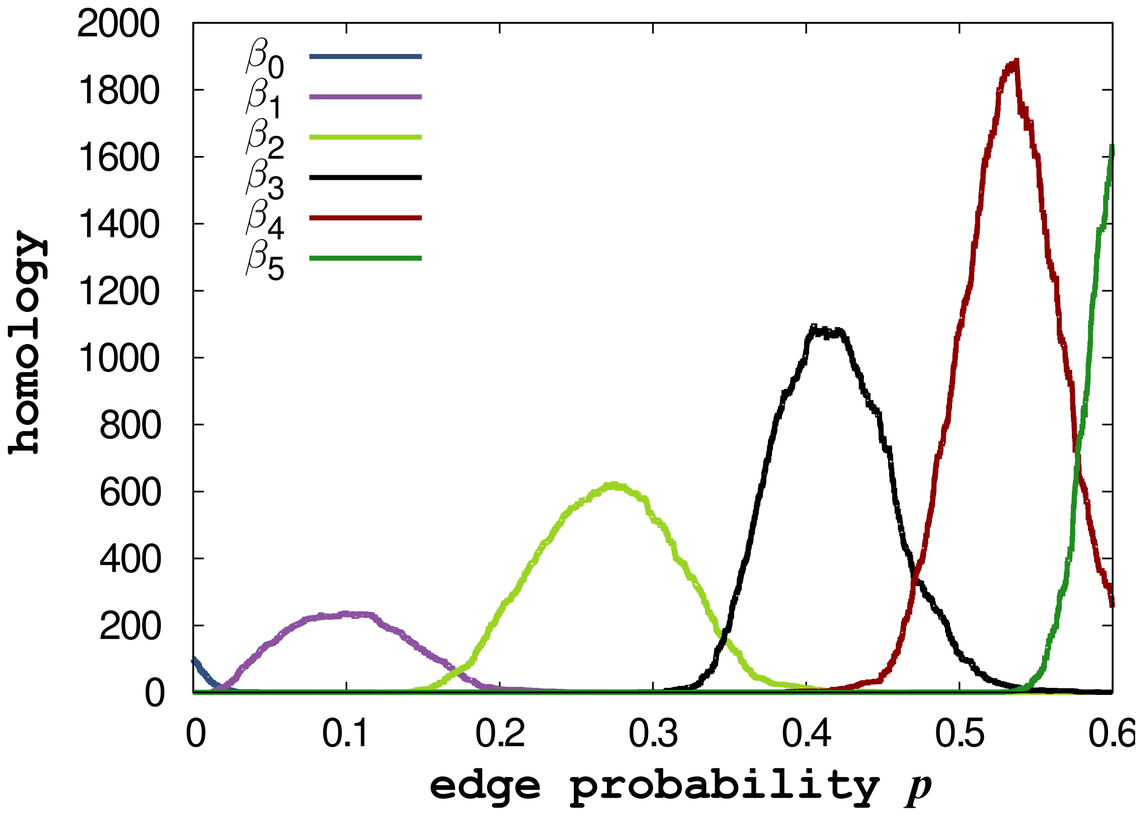
Random Flag complexes



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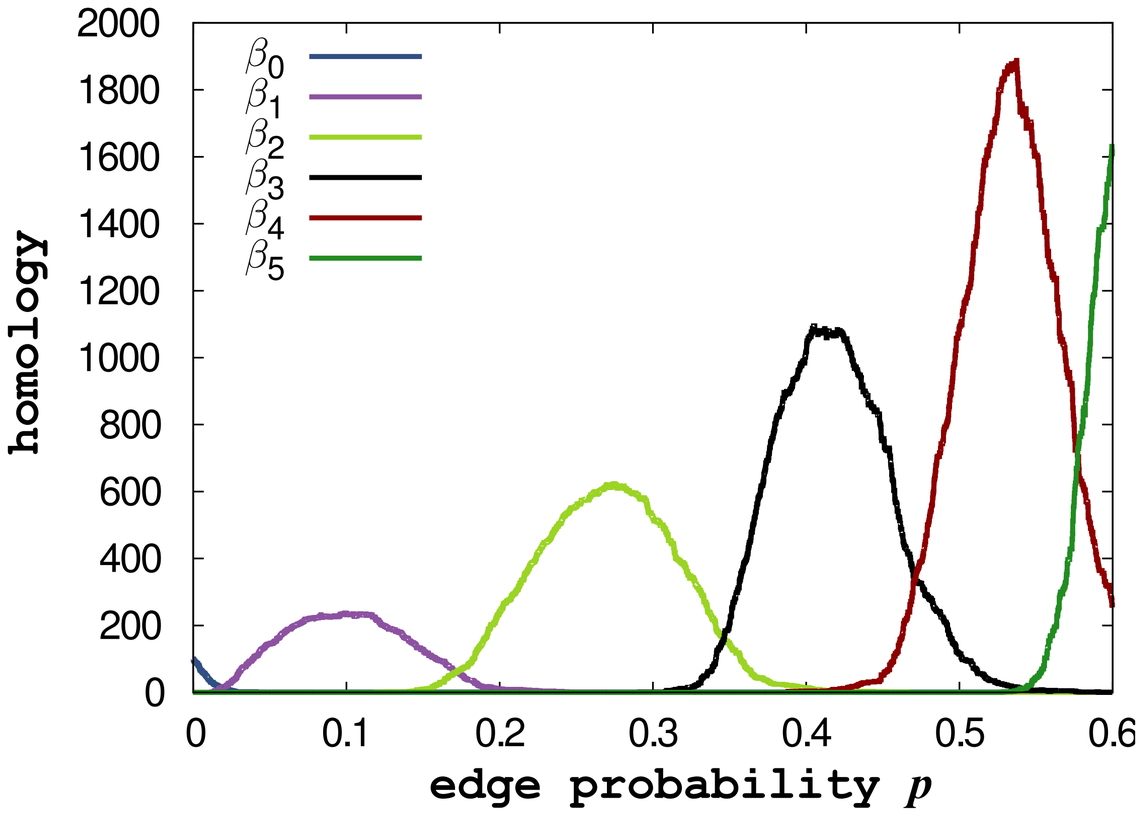

$$p(k) = [(k-1)N]^{-1/(k-1)}$$

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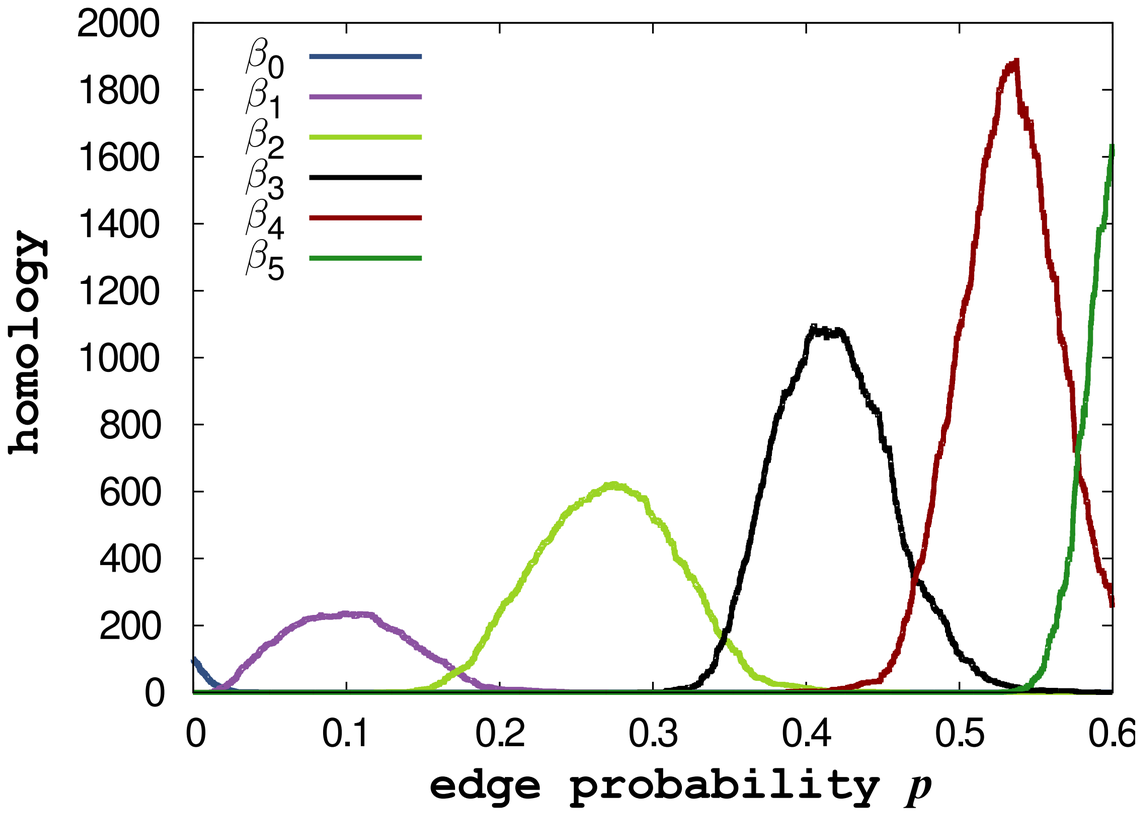

K-clique percolation thresholds

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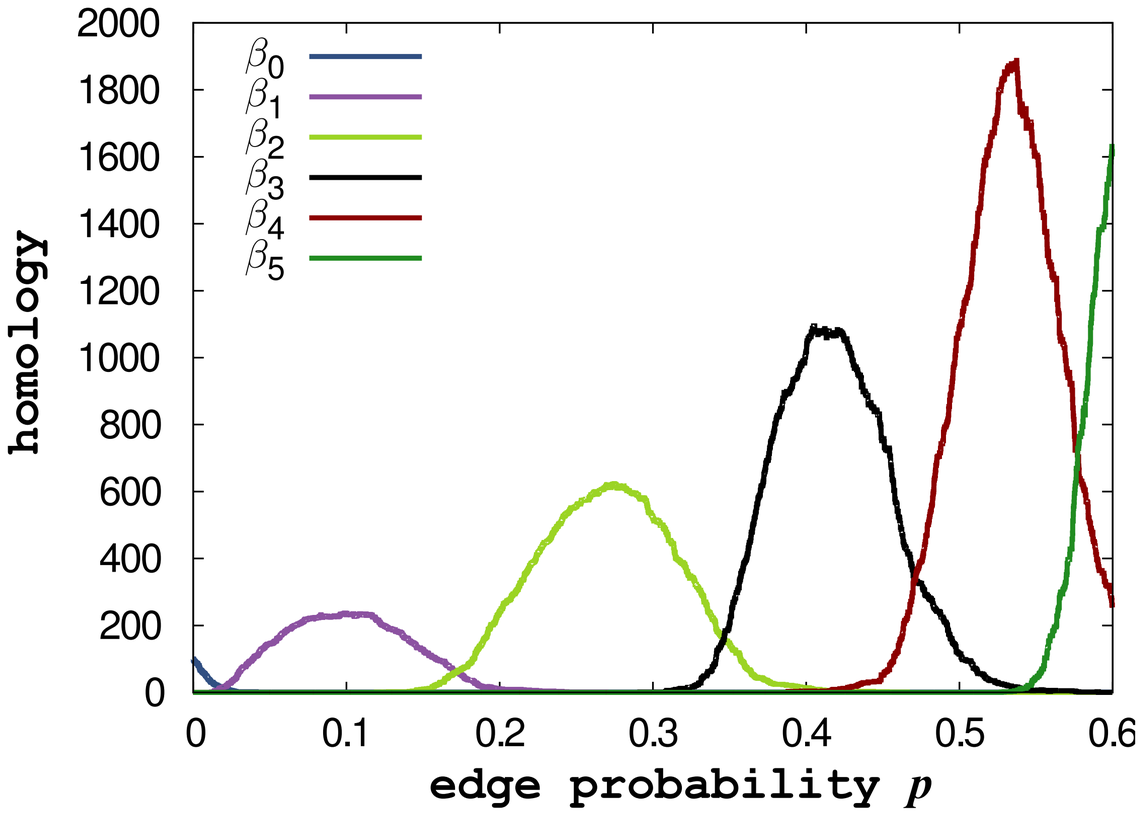

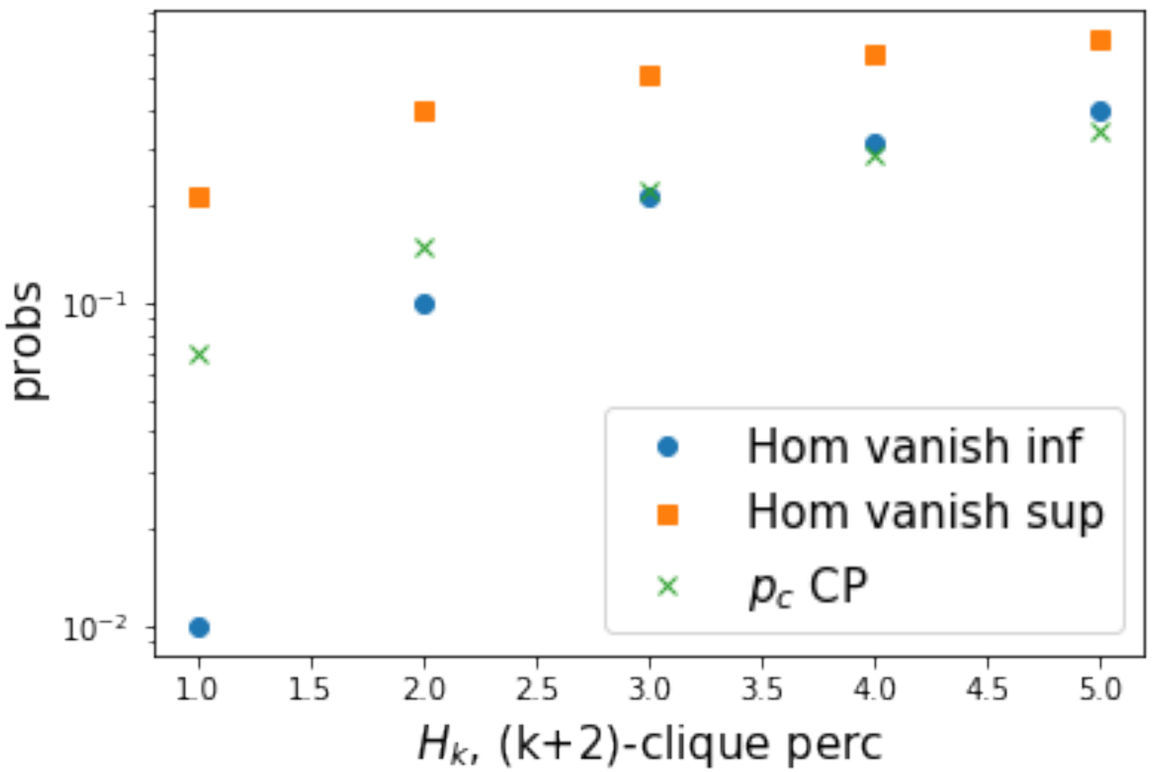

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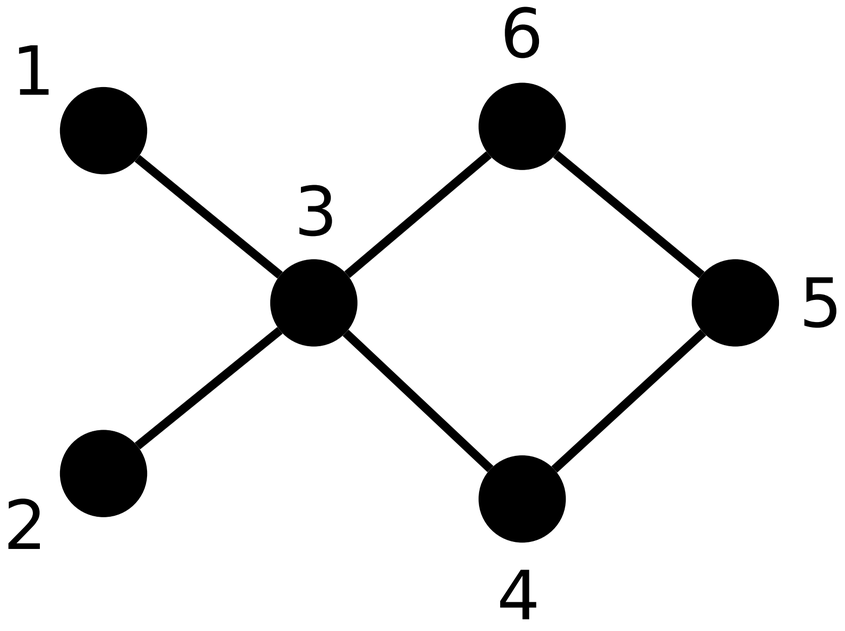
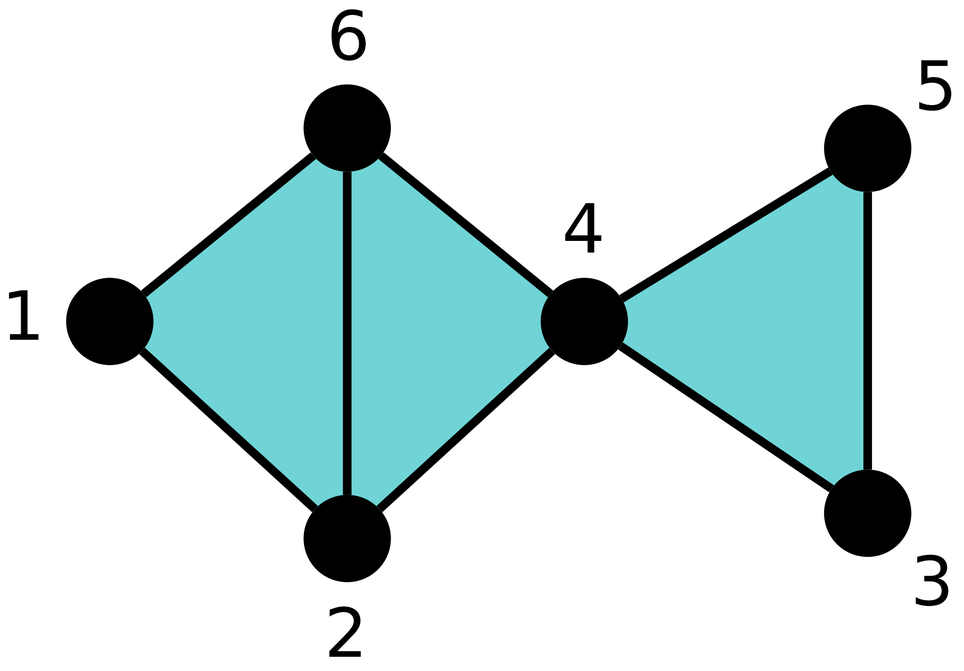
Courtney-Bianconi model

d-regular simplicial configuration model





d-regular simplicial configuration model taster

CANONICAL ENSEMBLE OF SIMPLICIAL COMPLEXES

Ensemble entropy

$$S = -\sum_G P(G) \ln P(G),$$

CM constraint

$$\overline{k_r} = \overline{k_{d,0}(r)} = \sum_G P(G) \sum_{\alpha \in \mathcal{Q}_d(N) | r \subset \alpha} a_\alpha.$$

Maximize….

$$\begin{aligned} \mathcal{F} \;=\; & S + \sum_{r=1}^{N} \lambda_r \left[\overline{k_r} - \sum_G P(G) k_{d,0}(r) \right] \\ & + \mu \left[1 - \sum_G P(G) \right], \end{aligned}$$

Generic solution….

$$P(G) = \frac{1}{Z} e^{-\sum_r \lambda_r k_{d,0}(r)}$$

$$Z = \prod_{\alpha \in \mathcal{Q}_d(N)} \left[1 + e^{-\sum_{r \subset \alpha} \lambda_r} \right].$$

d-regular simplicial configuration model taster

CANONICAL ENSEMBLE OF SIMPLICIAL COMPLEXES

Solve for degrees and substitute…

$$\overline{k_r} = \sum_{\alpha \in \mathcal{Q}_d(N) | r \subset \alpha} \frac{e^{-\sum_{m \subset \alpha} \lambda_m}}{1 + e^{-\sum_{m \subset \alpha} \lambda_m}}.$$

Why is this nice?

$$p_\alpha = \sum_G P(G) a_\alpha = \frac{e^{-\sum_{r \subset \alpha} \lambda_r}}{1 + e^{-\sum_{r \subset \alpha} \lambda_r}}$$

Instance probability

$$P(G) = \prod_{\alpha \in \mathcal{Q}_d(N)} \left[p_\alpha^{a_\alpha} (1 - p_\alpha)^{1 - a_\alpha} \right]$$

Full entropy expression

$$S = - \sum_{\alpha \in \mathcal{Q}_d(N)} \left[p_\alpha \ln p_\alpha + (1 - p_\alpha) \ln(1 - p_\alpha) \right]$$

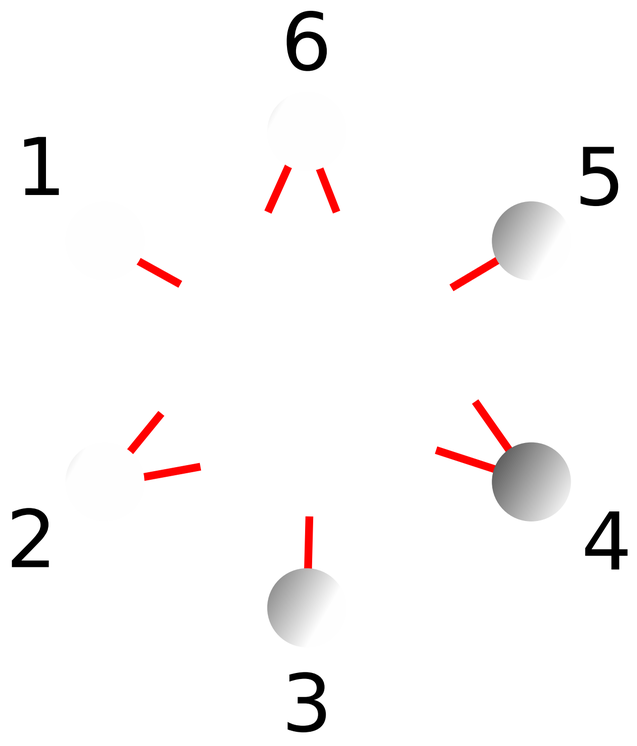
d-regular simplicial configuration model

Generalized network structures:
The configuration model and the canonical ensemble of simplicial complexes

Owen T. Courtney[1] and Ginestra Bianconi[1]
[1]*School of Mathematical Sciences, Queen Mary University of London, E1 4NS, London, UK*

Very pretty —sed dense— paper, hence…

d-regular simplicial configuration model



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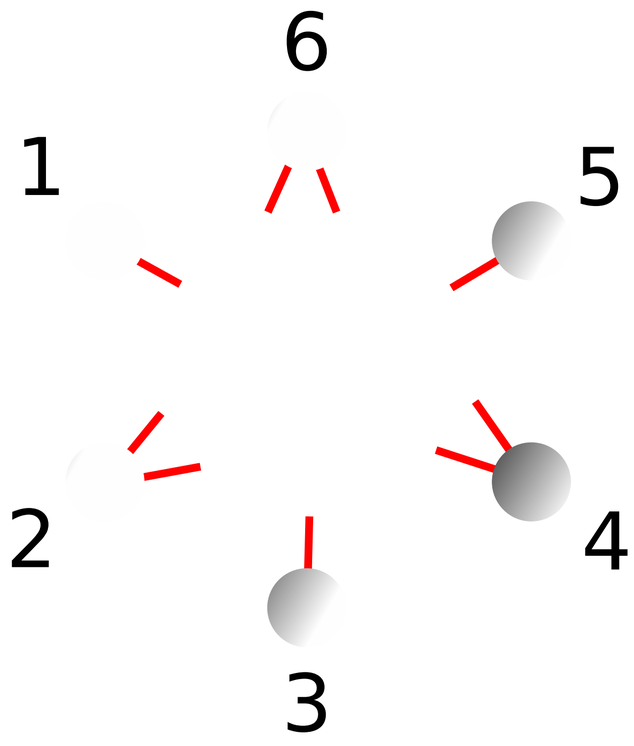

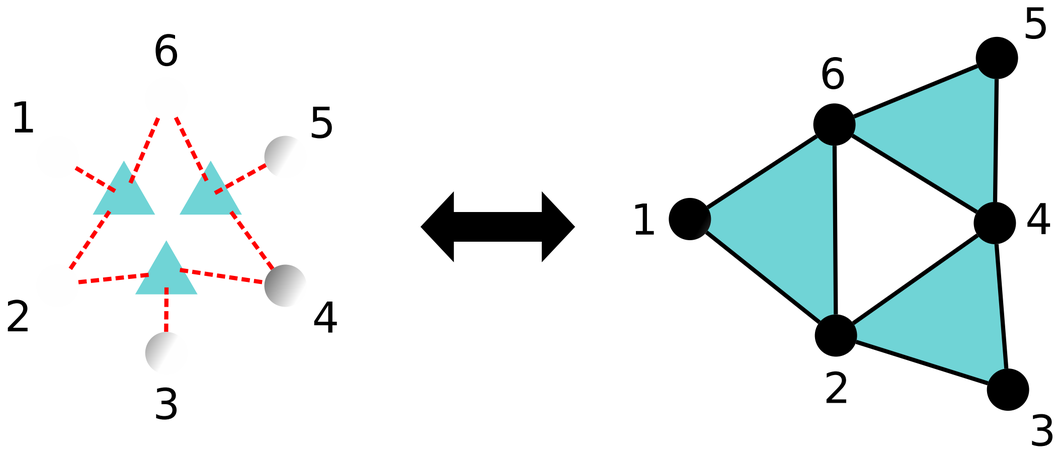

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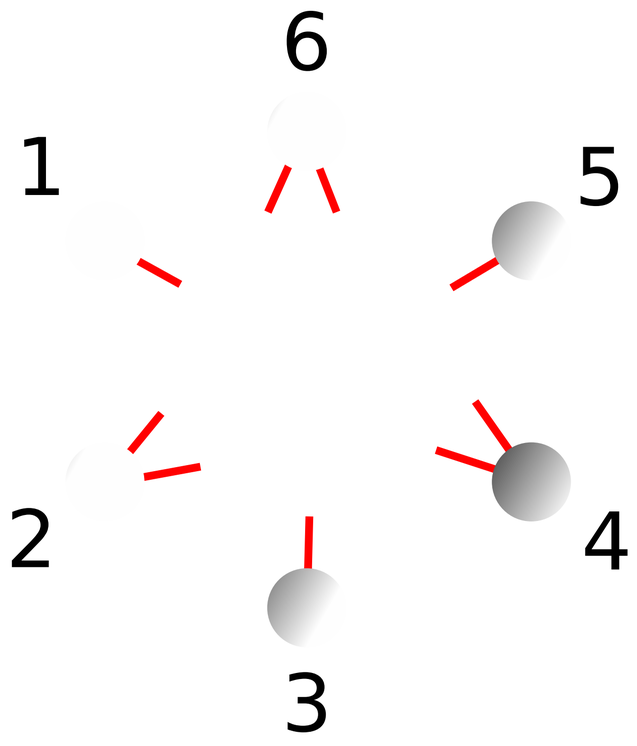

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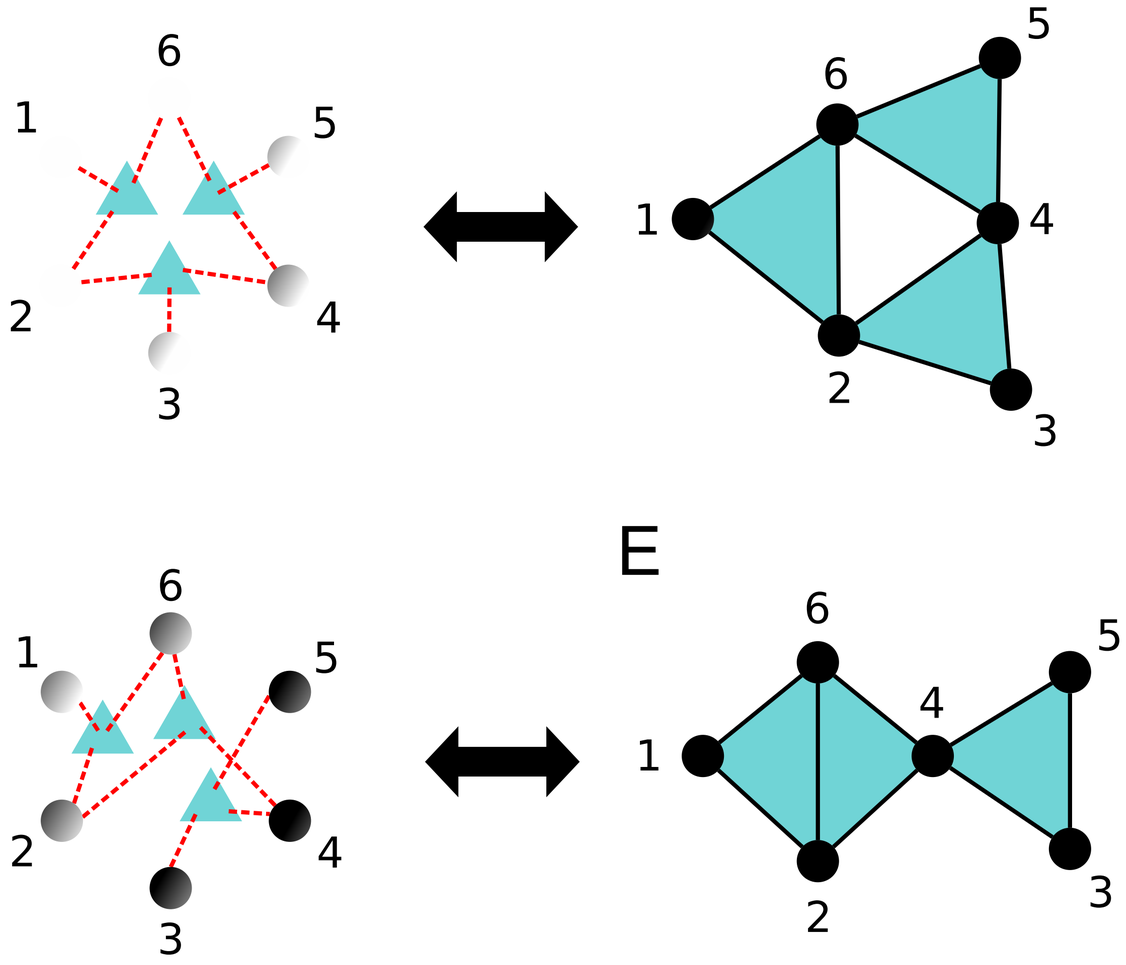

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d-regular simplicial configuration model taster

CONFIGURATION MODEL FOR SIMPLICIAL COMPLEXES

Instance probability

$$P(G) = \frac{1}{\mathcal{N}} \prod_{r=1,N} \delta(k_r, k_{d,0}(r)).$$

CM constraint

$$\mathcal{N} = \sum_G \prod_{r=1,N} \delta(k_r, k_{d,0}(r)).$$

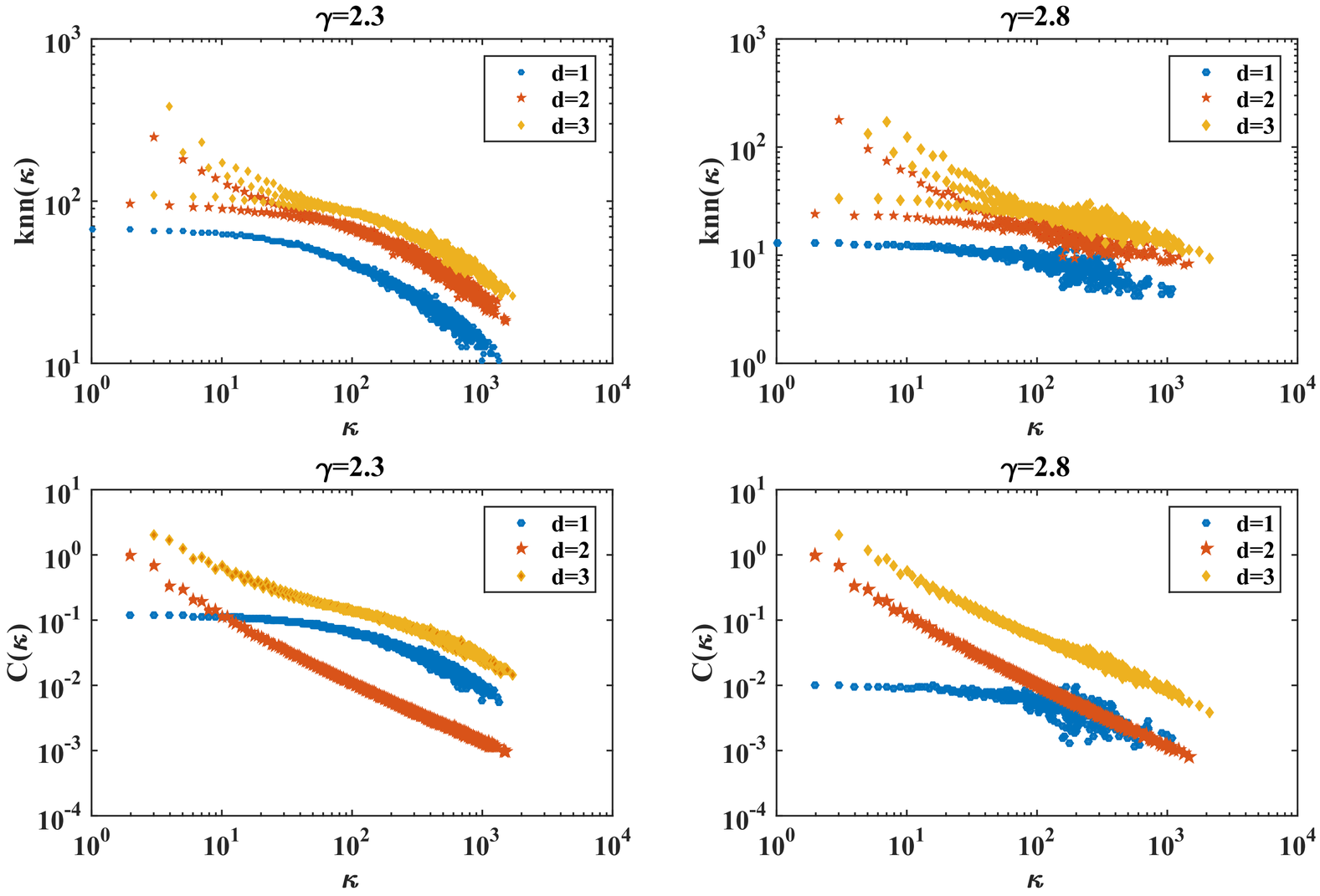
Ensemble entropy

$$\Sigma = \ln \mathcal{N} = \ln \left[\sum_G \prod_r \delta\left(k_r, k_{d,0}(r)\right) \right].$$

$$\Omega = -\ln \left[\sum_G P(G) \prod_r \delta\left(k_r, k_{d,0}(r)\right) \right],$$

$$\Sigma = S - \Omega$$

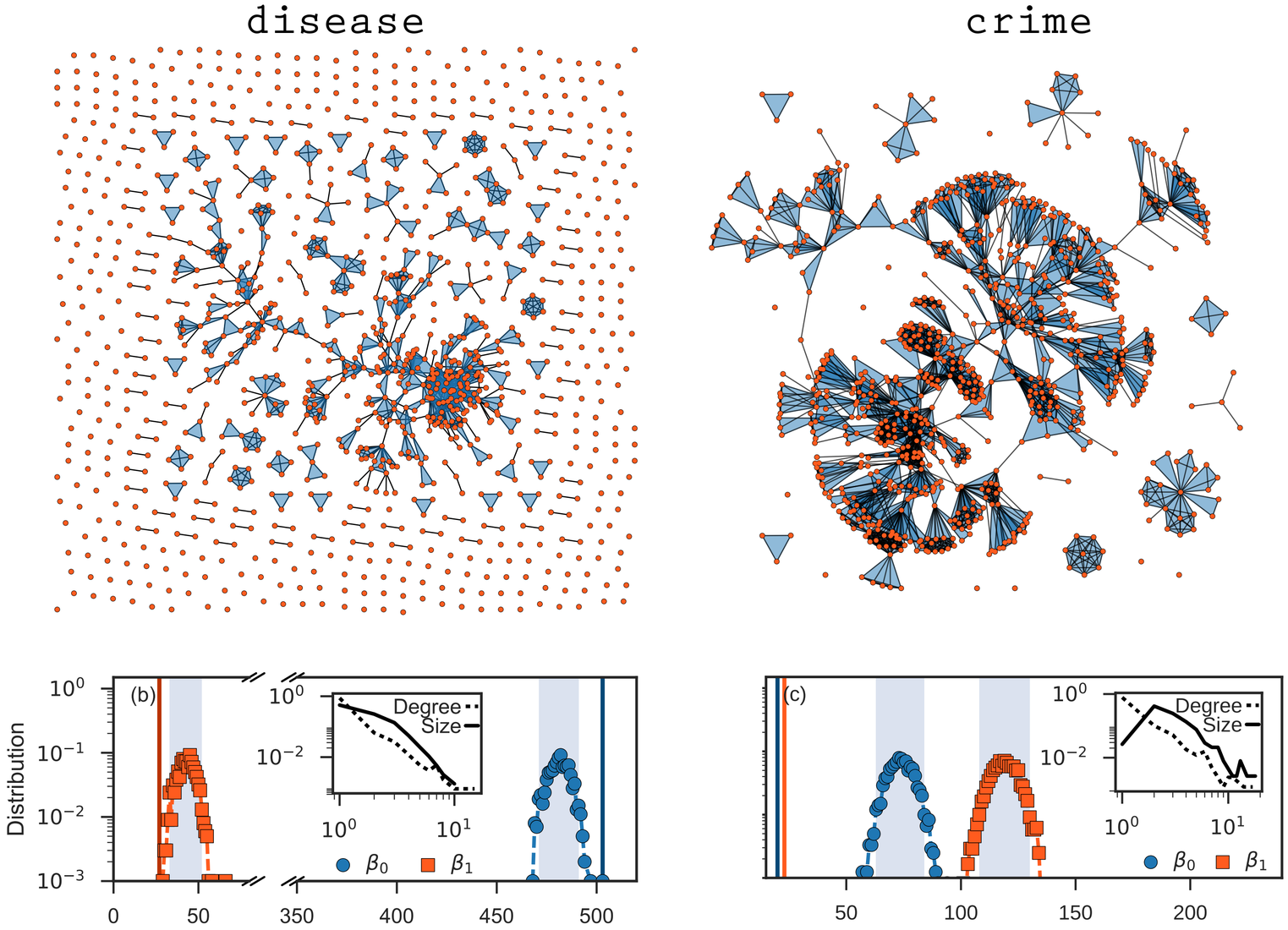
d-regular simplicial configuration model



Notebook

Simplicial Configuration Model

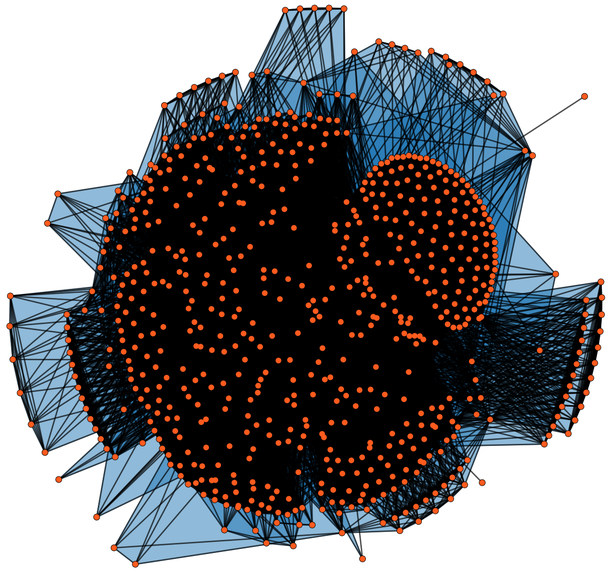
Homology as significant structure

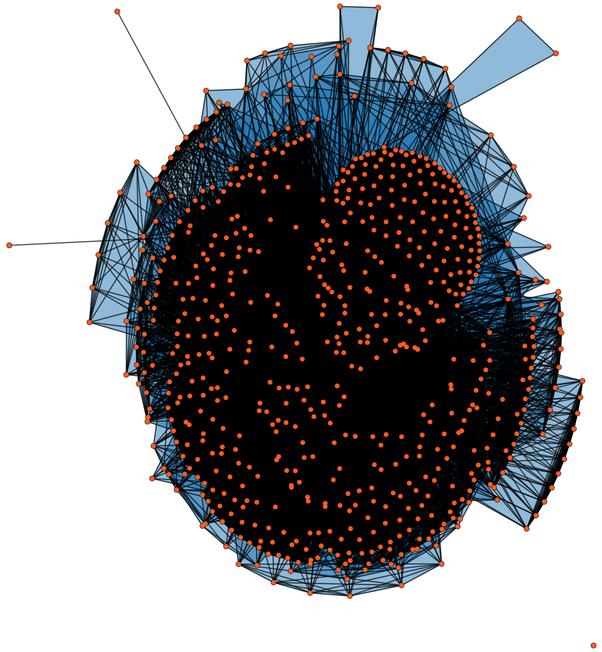


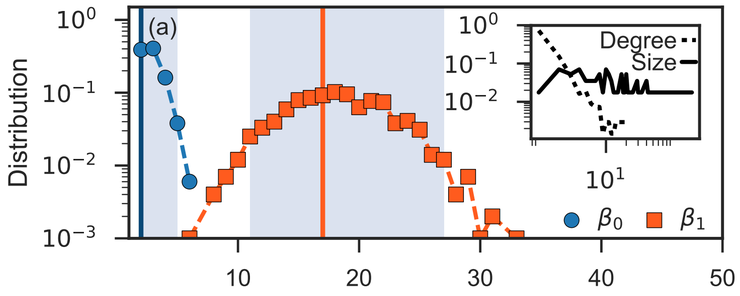
ean-Gabriel, et al. "Construction of and efficient sampling from the simplicial configuration model." arXiv preprint arXiv:1705.10298 (2017)

Homology as significant structure

pollinators







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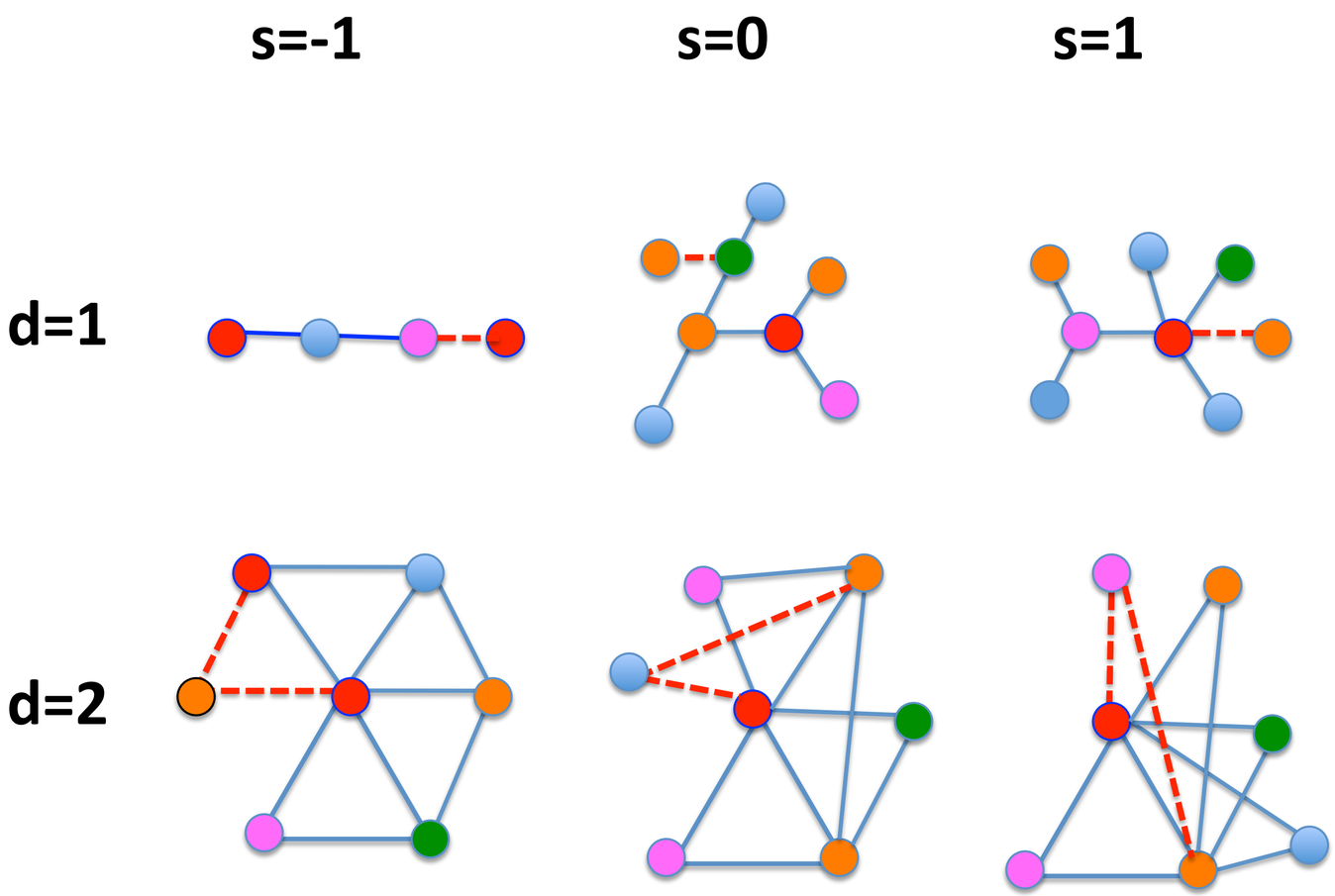
Growing simplicial complexes

Network geometry with flavour

$$\Pi_\alpha^{[s]} = \frac{1}{Z^{[s]}(t)} e^{-\beta\epsilon_\alpha}(1+sn_\alpha),$$

$$n_\alpha = k_{d,d-1}(\alpha) - 1.$$

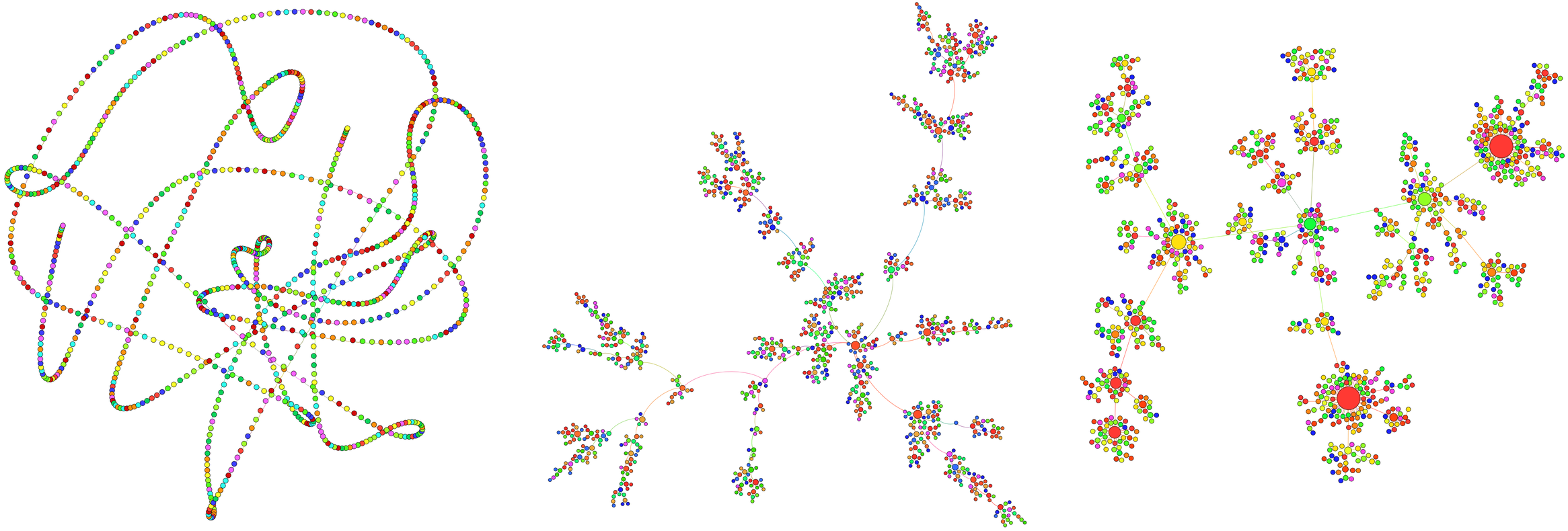
$$Z^{[s]}(t) = \sum_{\alpha\in\mathcal{S}_{d,d-1}} e^{-\beta\epsilon_\alpha}(1+sn_\alpha).$$



Network geometry with flavor: from complexity to quantum geometry

Ginestra Bianconi[1] and Christoph Rahmede[2]
[1] *School of Mathematical Sciences, Queen Mary University of London, London E1 4NS, United Kingdom*
[2] *Rome International Centre for Material Science Superstripes RICMASS, via dei Sabelli 119A, 00185 Roma, Italy*

Network geometry with flavour

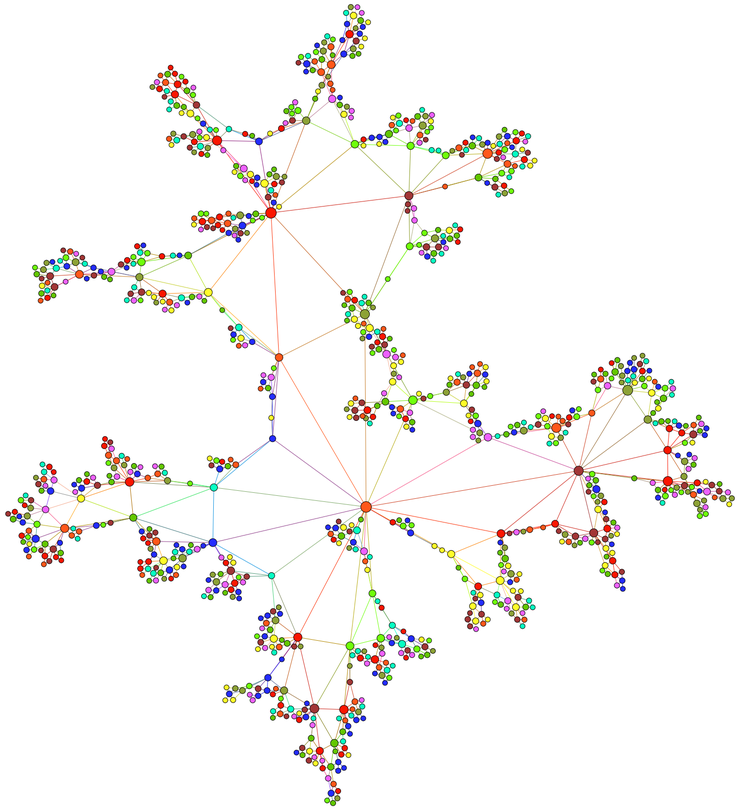


(a)
d = 1, s=-1

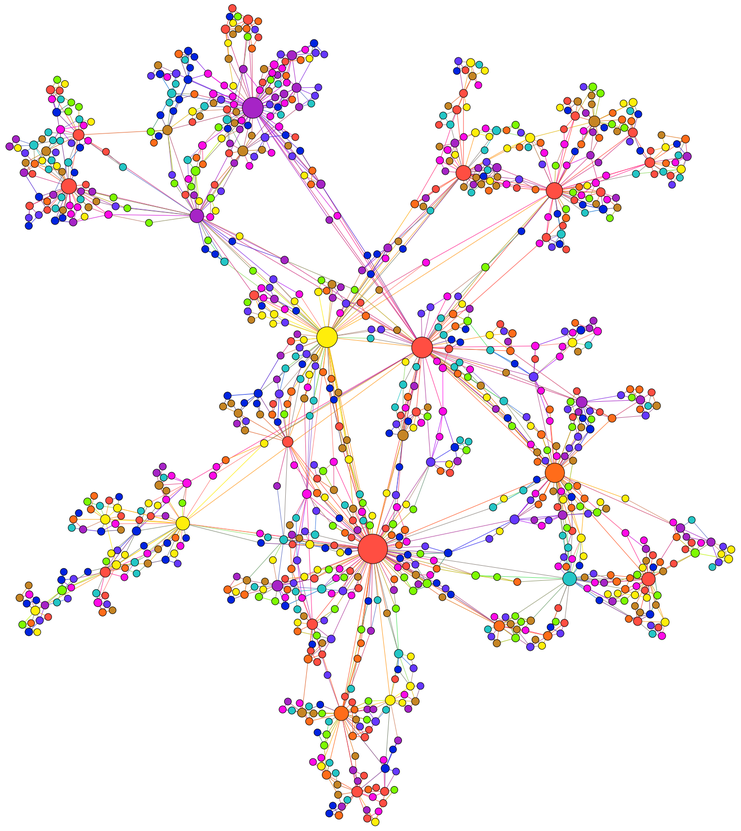
(b)
d = 1, s = 0

(c)
d = 1, s = 1

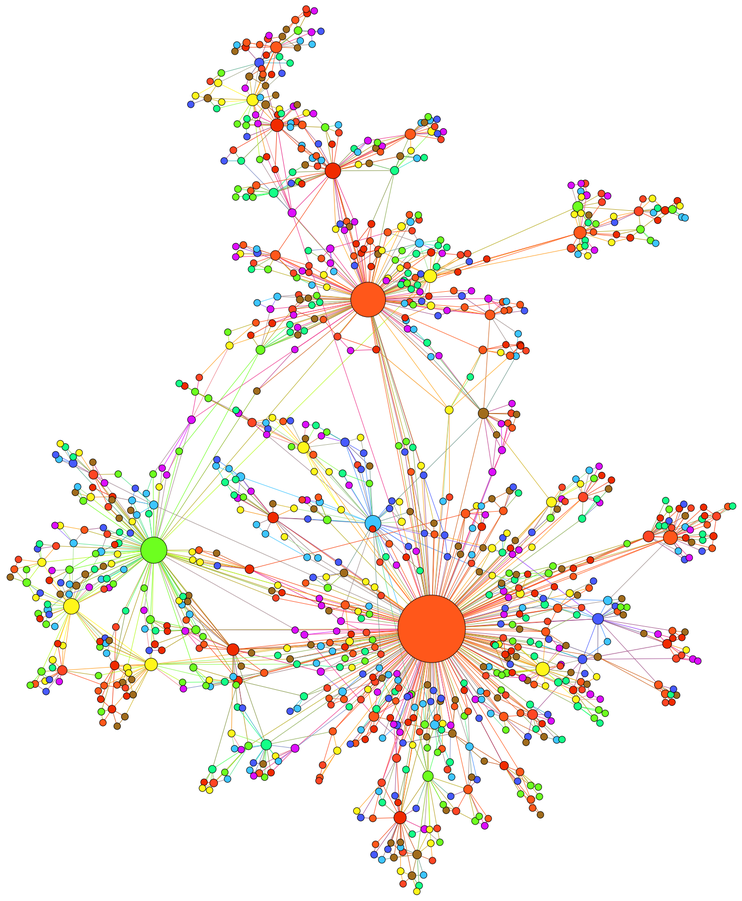
Network geometry with flavour



(d)
d = 2, s = -1

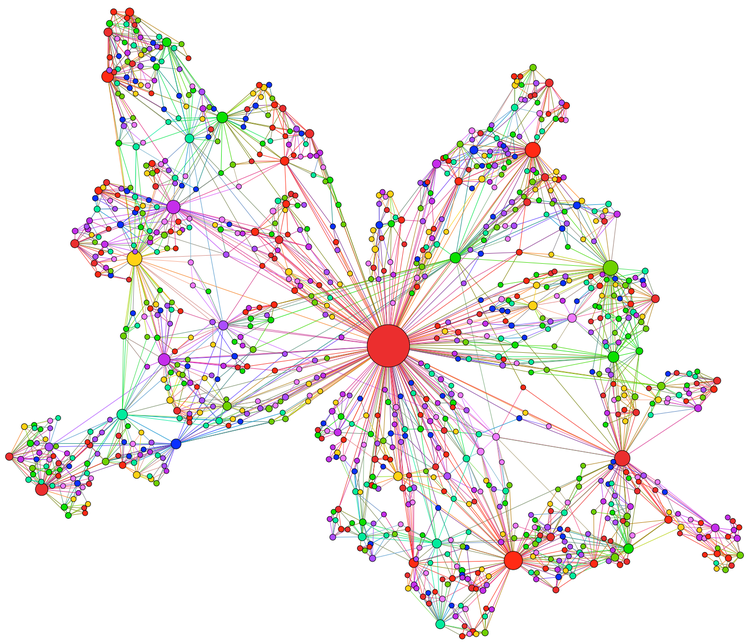


(e)
d = 2, s = 0



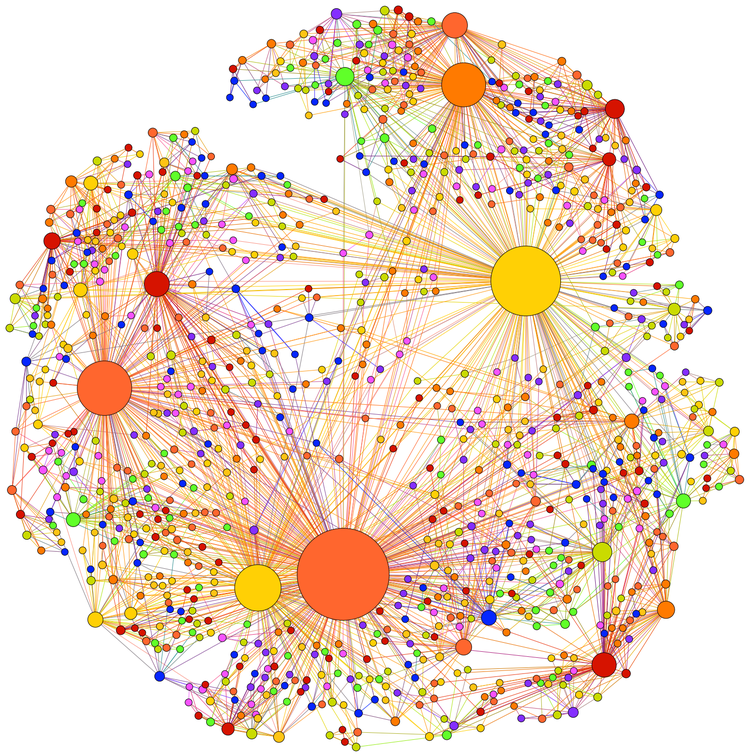
(f)
d = 2, s = 1

Network geometry with flavour



(g)
d = 3, s = -1

(h)
d = 3, s = 0



(i)
d = 3, s = 1

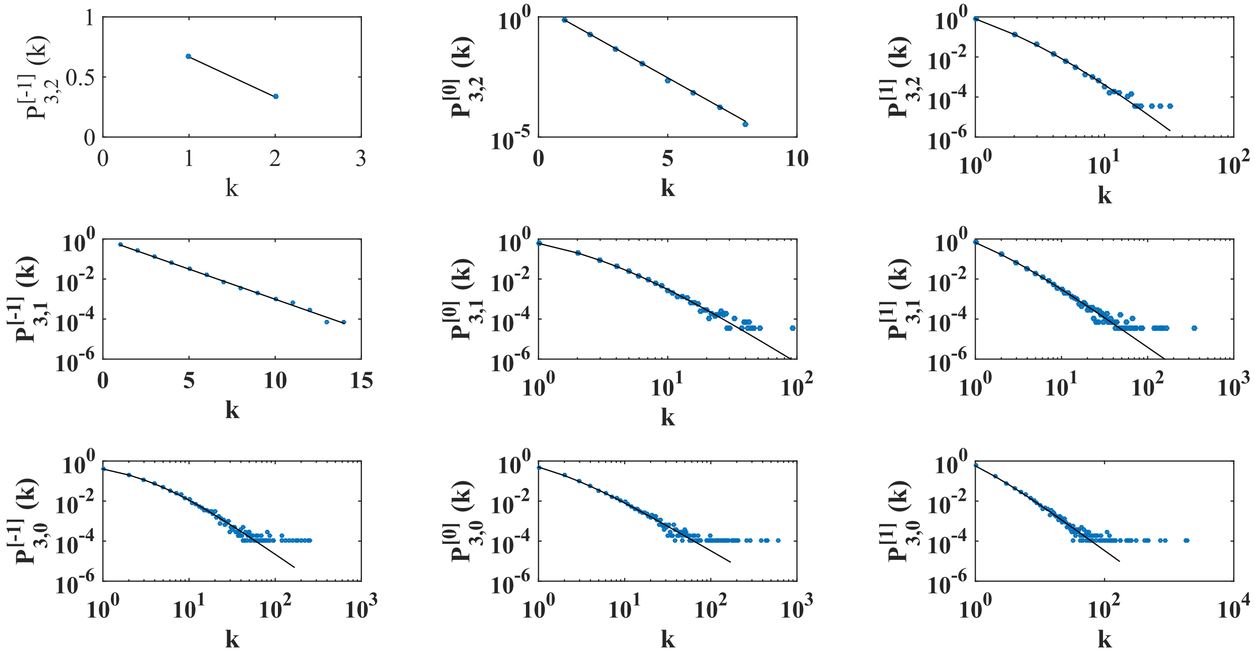
Network geometry with flavour

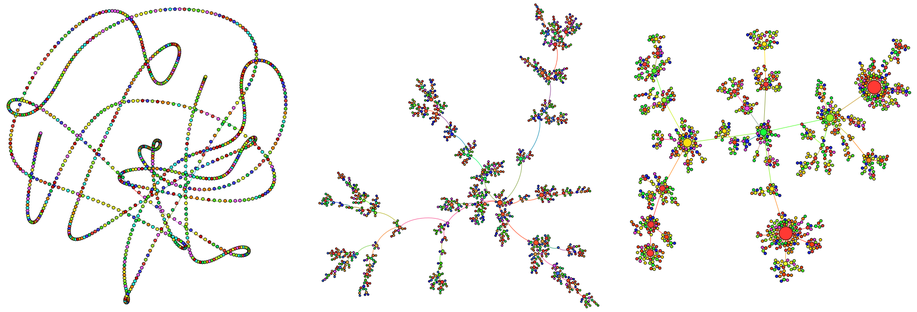
TABLE I: Distribution of generalized degrees of faces of dimension δ in a d-dimensional NGF of flavor s at $\beta = 0$. For $d \geq d_c^{[\delta,s]} = 2(\delta+1) - s$ the power-law distributions are scale-free, i.e. the second moment of the distribution diverges.

flavor	$s=-1$	$s=0$	$s=1$
$\delta = d-1$	Binomial	Exponential	Power-law
$\delta = d-2$	Exponential	Power-law	Power-law
$\delta \leq d-3$	Power-law	Power-law	Power-law

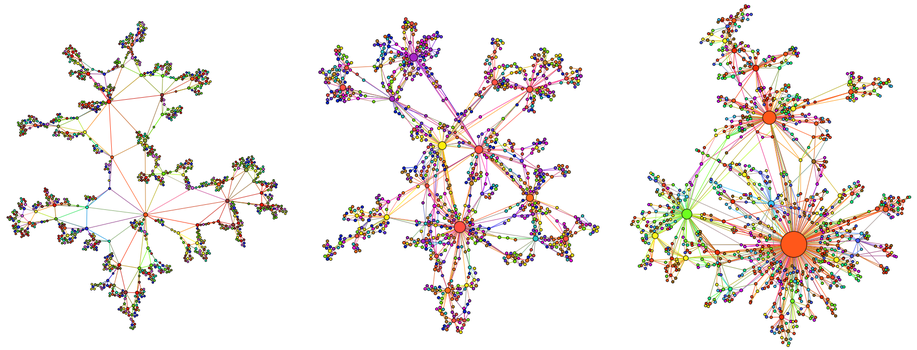
TABLE II: The average $\langle k_{d,\delta} - 1 | \epsilon, s \rangle$ of the generalized degrees $k_{d,\delta}$ of δ-faces with energy ϵ minus one in a d-dimensional NGF of flavor s follows either the Fermi-Dirac, the Boltzmann or the Bose-Einstein statistics depending on the values of the dimensions d and δ.

flavor	$s=-1$	$s=0$	$s=1$
$\delta = d-1$	Fermi-Dirac	Boltzmann	Bose-Einstein
$\delta = d-2$	Boltzmann	Bose-Einstein	Bose-Einstein
$\delta \leq d-3$	Bose-Einstein	Bose-Einstein	Bose-Einstein

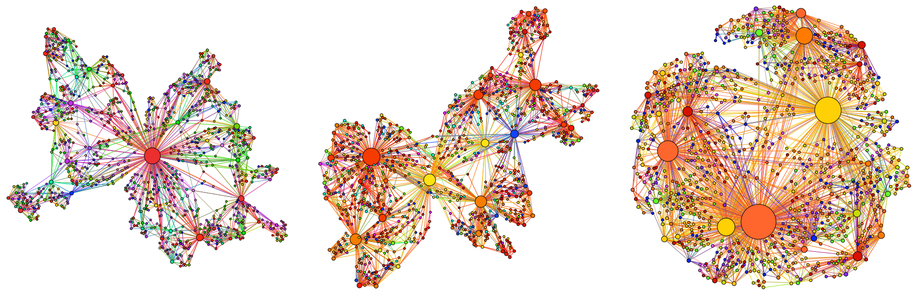




(a) d = 1, s=-1 (b) d = 1, s = 0 (c) d = 1, s = 1

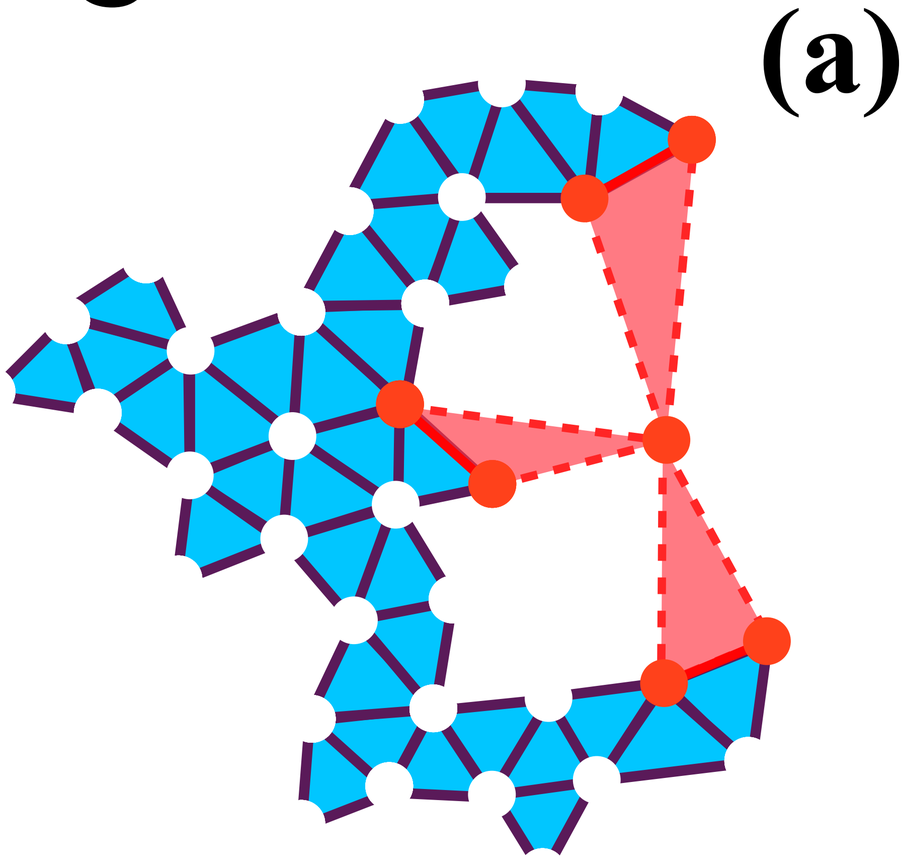


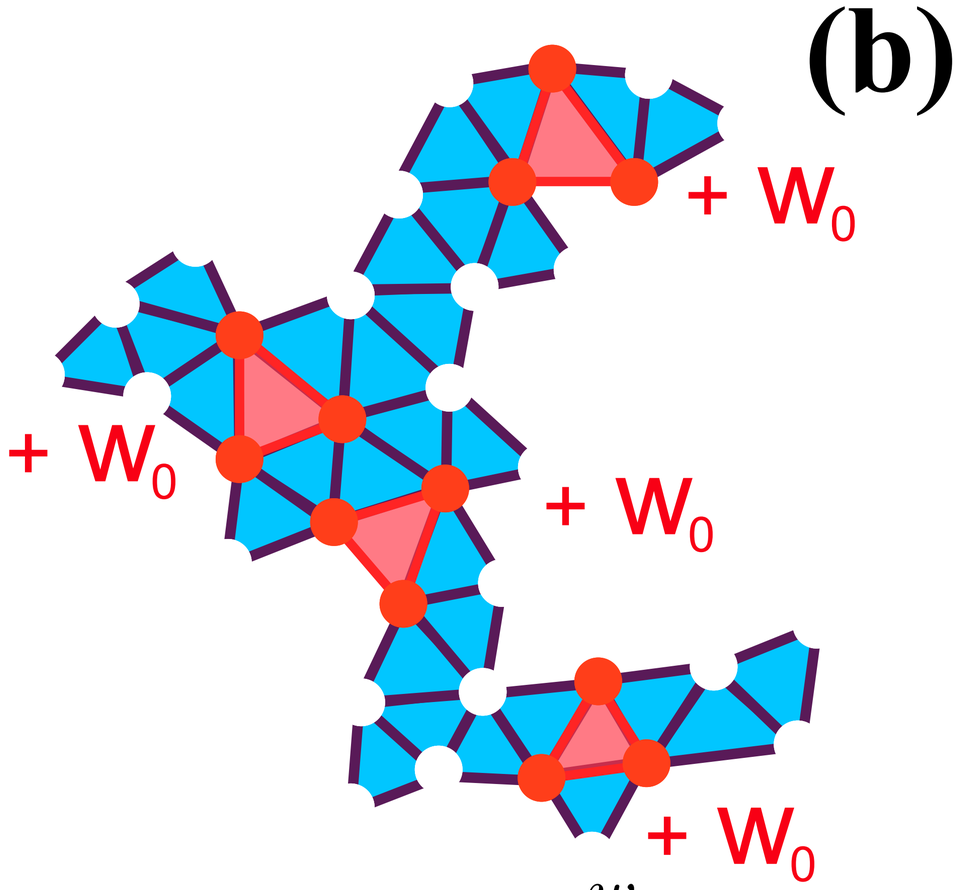
(d) d = 2, s = -1 (e) d = 2, s = 0 (f) d = 2, s = 1



(g) d = 3, s = -1 (h) d = 3, s = 0 (i) d = 3, s = 1

Weighted GRSC





$$\Pi_{d-1}(\alpha) = \frac{1}{\mathcal{Z}_t}(1 + s n_\alpha),$$

$$n_\alpha = k^\alpha_{d,d-1} - 1 \qquad s = -1, 0, 1$$

$$\tilde{\Pi}_d(\alpha) = \frac{w_\alpha}{\tilde{\mathcal{Z}}_t},$$

$$(\#a, \#b) = (m, m')$$

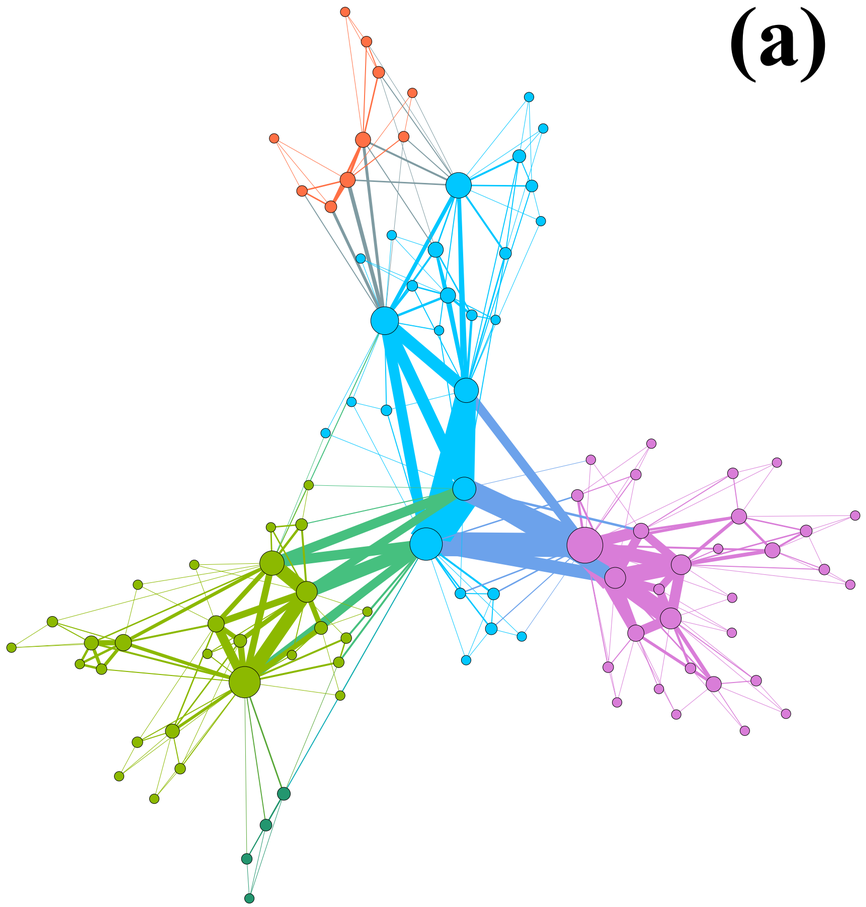
Weighted Growing Simplicial Complexes

Owen Courtney[1] and Ginestra Bianconi[1]

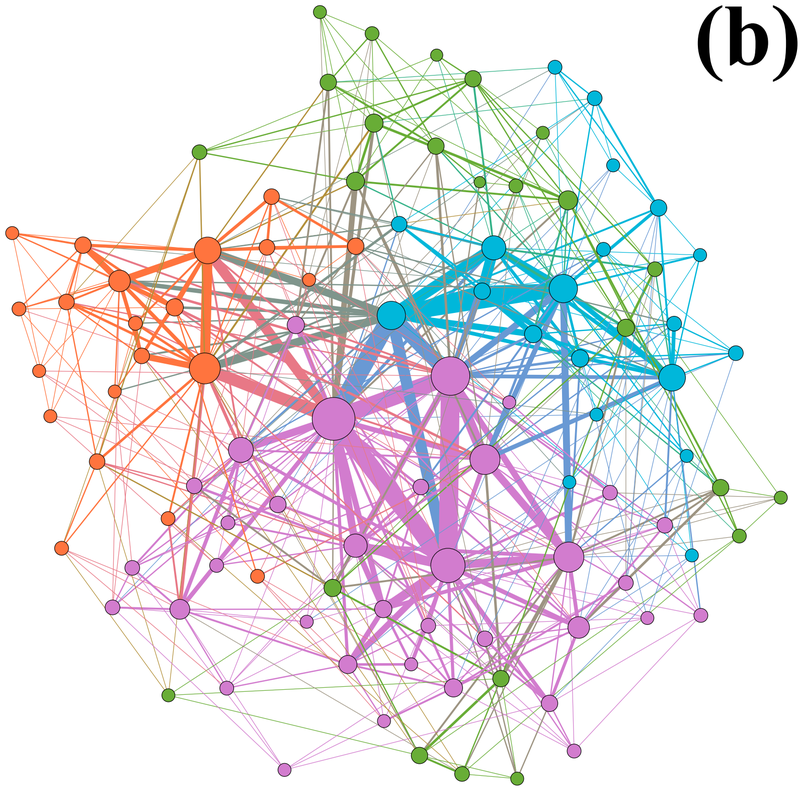
[1]*School of Mathematical Sciences, Queen Mary University of London, E1 4NS, London, UK*

Weighted GRSC

$(m, m') = (1, 2)$



$(m, m') = (2, 1)$



Weighted GRSC

$$k_{d,\delta}(t,t_\alpha) = \begin{cases} c_\delta \frac{d-\delta}{d+s-\delta-1}\left(\frac{t}{t_\alpha}\right)^{\lambda_\delta} + c_\delta \frac{s-1}{d+s-\delta-1} & \text{for} \quad \delta - s \neq d-1, \\ c_\delta \frac{1-s}{d+s}\log\left(\frac{t}{t_\alpha}\right) + c_\delta & \text{for} \quad \delta - s = d-1, \end{cases}$$

$$\lambda_\delta = \frac{d+s-\delta-1}{d+s}.$$

$$c_\delta = \begin{cases} 1 & \text{for} \quad \delta > 0, \\ m & \text{for} \quad \delta = 0. \end{cases}$$

$$\lambda = \frac{m'}{m+m'}.$$

$$s_{d,\delta}(t,t_\alpha) \propto \begin{cases} \left(\frac{t}{t_\alpha}\right)^{\lambda_\delta} & \text{if} \quad \lambda < \lambda_\delta, \\ \left(\frac{t}{t_\alpha}\right)^{\lambda} & \text{if} \quad \lambda > \lambda_\delta, \\ \left(\frac{t}{t_\alpha}\right)^{\lambda}\log\left(\frac{t}{t_\alpha}\right) & \text{if} \quad \lambda = \lambda_\delta. \end{cases}$$

$$s_{d,\delta}(k_{d,\delta}) \propto \begin{cases} k_{d,\delta} & \text{for} \quad \lambda < \lambda_\delta, \\ k_{d,\delta}\ln k_{d,\delta} & \text{for} \quad \lambda = \lambda_\delta, \\ (k_{d,\delta})^{\lambda/\lambda_\delta} & \text{for} \quad \lambda > \lambda_\delta. \end{cases}$$

$$s_{d,\delta}(k_{d,\delta}) \propto e^{\beta k_{d,\delta}}, \qquad \beta = \lambda \frac{d+s}{(1-s)c_\delta}.$$

Questions?
Emotional support?