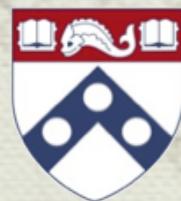


Extracting Hidden Hierarchies in Weighted Distribution Networks

Eleni Katifori

Department of Physics and Astronomy, University of Pennsylvania
and

Max Planck Institute of Dynamics and Self-Organization, Goettingen



Penn

Physics & Astronomy



MAX-PLANCK-GESELLSCHAFT

Many thanks to:



| | |
|-----------------------|-----------------------------|
| Douglas Daly | (New York Botanical Garden) |
| Marcelo Magnasco | (Rockefeller NY) |
| Carl Modes | (Rockefeller NY) |
| Jana Lasser | (MPI DS) |
| Henrik Ronellenfitsch | (MPI DS) |

| Number of variables → | | | | |
|-----------------------|---|--|--|--|
| | $n = 1$ | $n = 2$ | $n \geq 3$ | $n \gg 1$ |
| Linear | <i>Growth, decay, or equilibrium</i> | <i>Oscillations</i> | | <i>Collective phenomena</i> |
| | Exponential growth | Linear oscillator | Civil engineering, structures | Coupled harmonic oscillators |
| | RC circuit | Mass and spring | Electrical engineering | Solid-state physics |
| | Radioactive decay | RLC circuit | | Molecular dynamics |
| Nonlinearity ↓ | | 2-body problem (Kepler, Newton) | | Equilibrium statistical mechanics |
| | | | | Quantum mechanics (Schrödinger, Heisenberg, Dirac) |
| | | | | Heat and diffusion |
| | | | | Acoustics |
| Nonlinear | | | | Viscous fluids |
| | | | <i>The frontier</i> | |
| | | | <i>Chaos</i> | |
| | Fixed points | Pendulum | Strange attractors (Lorenz) | Coupled nonlinear oscillators |
| | Bifurcations | Anharmonic oscillators | | Lasers, nonlinear optics |
| | Overdamped systems, relaxational dynamics | Limit cycles | 3-body problem (Poincaré) | Nonequilibrium statistical mechanics |
| | Logistic equation for single species | Biological oscillators (neurons, heart cells) | Chemical kinetics | Nonlinear solid-state physics (semiconductors) |
| | | Predator-prey cycles | Iterated maps (Feigenbaum) | Quantum field theory |
| | | Nonlinear electronics (van der Pol, Josephson) | Fractals (Mandelbrot) | Reaction-diffusion, biological and chemical waves |
| | | | Forced nonlinear oscillators (Levinson, Smale) | Fibrillation |
| | | | Practical uses of chaos | Epilepsy |
| | | | Quantum chaos ? | Turbulent fluids (Navier-Stokes) |
| | | | | Life |

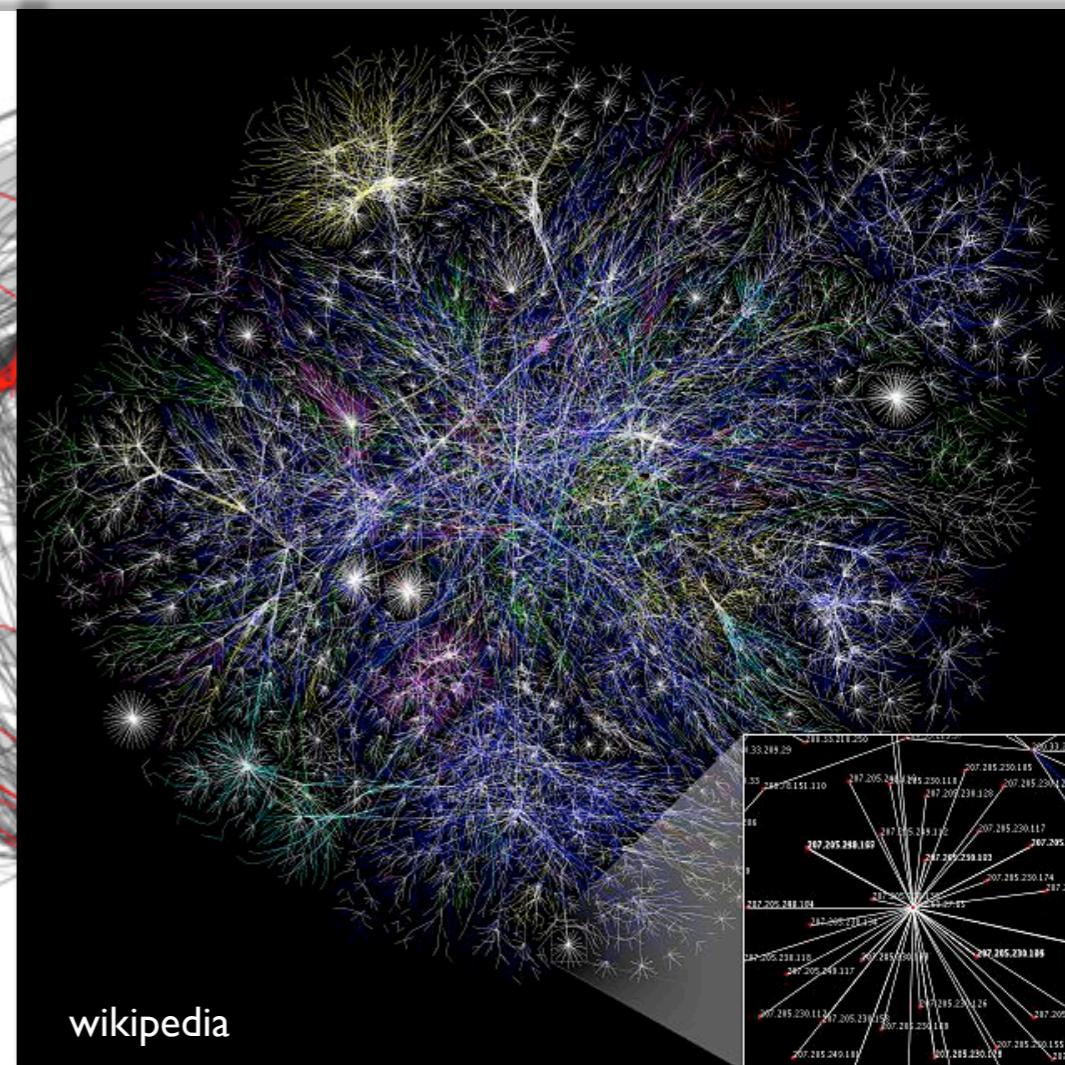
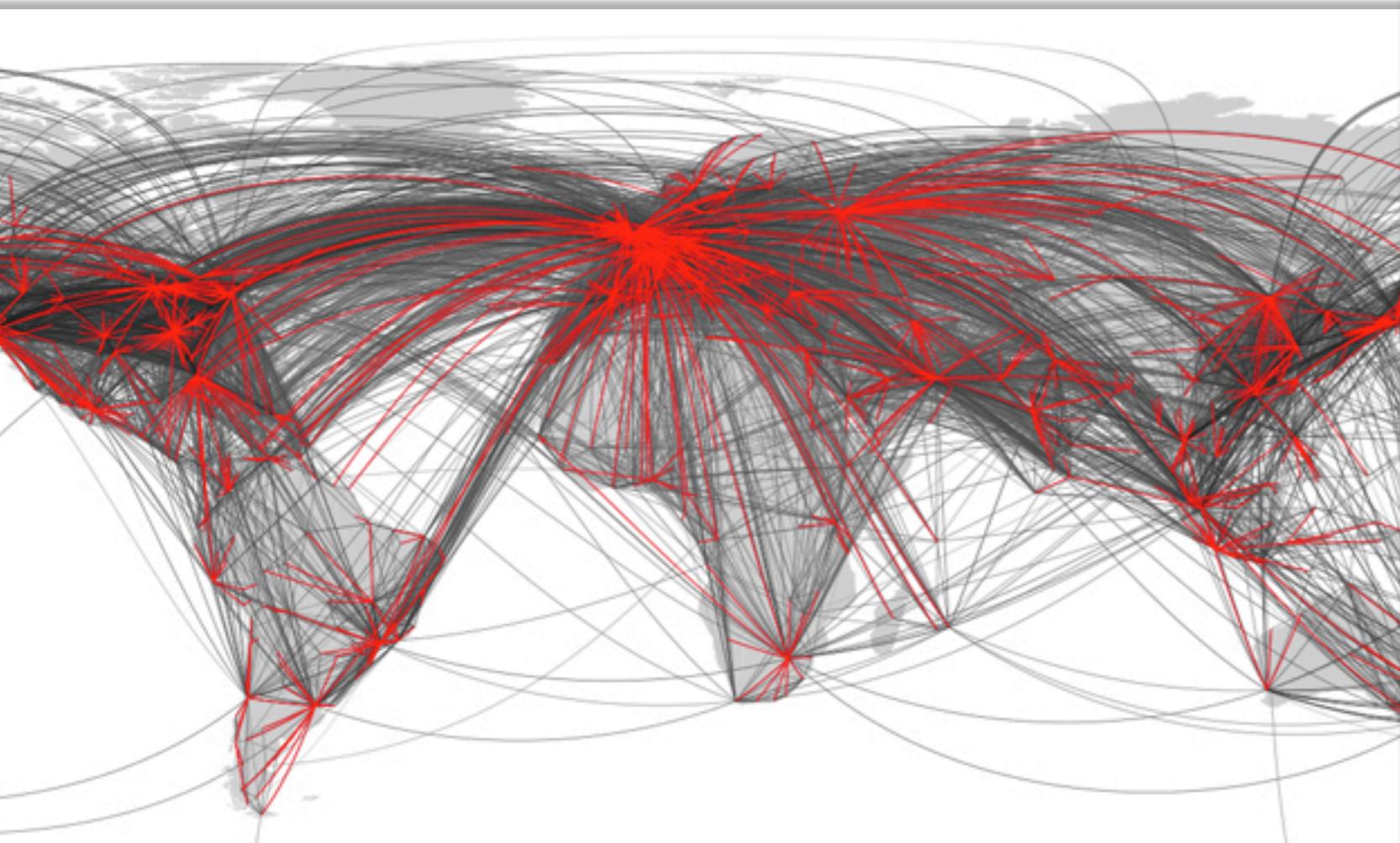
Graph morphometrics

How can one quantify a complex graph?

3d Networks with **unrestricted** degree

Internet, airports, neuronal networks in the brain,
social networks...

*scale free,
clustering coefficients,
degree distributions,
hubs...*

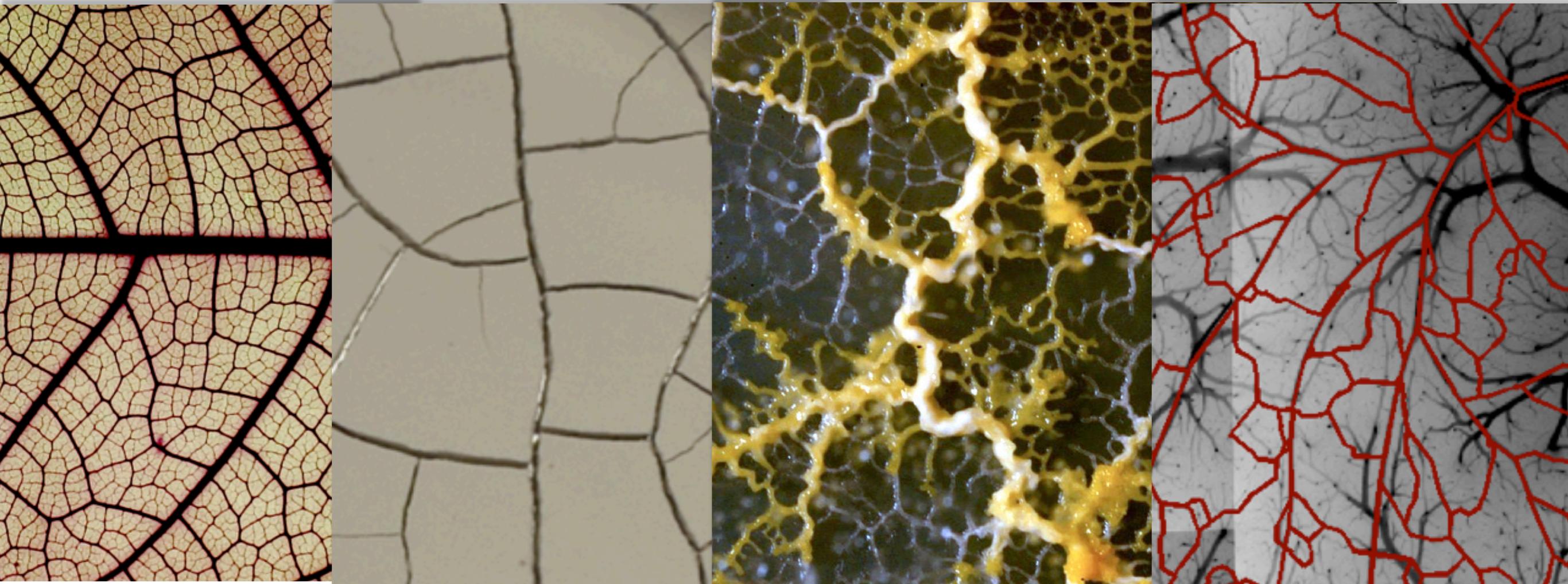


Graph morphometrics

How can one quantify a complex graph?

2d Networks with **restricted** degree

Leaf vascular networks, crack patterns, road networks...



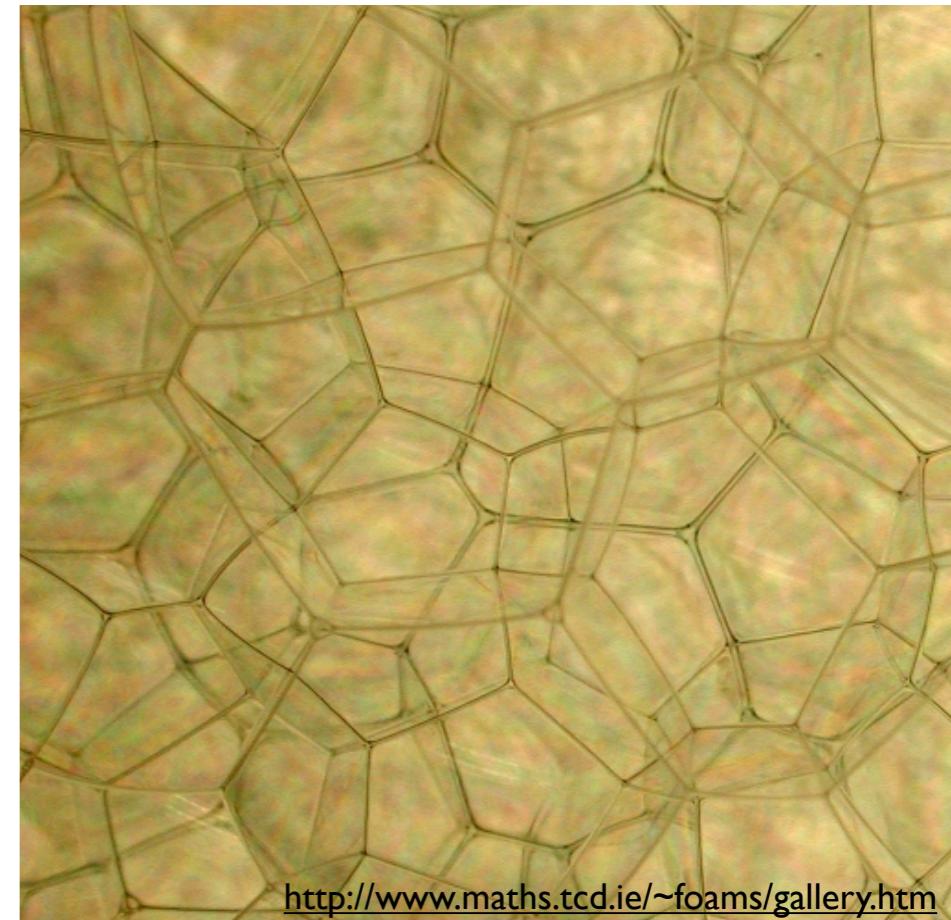
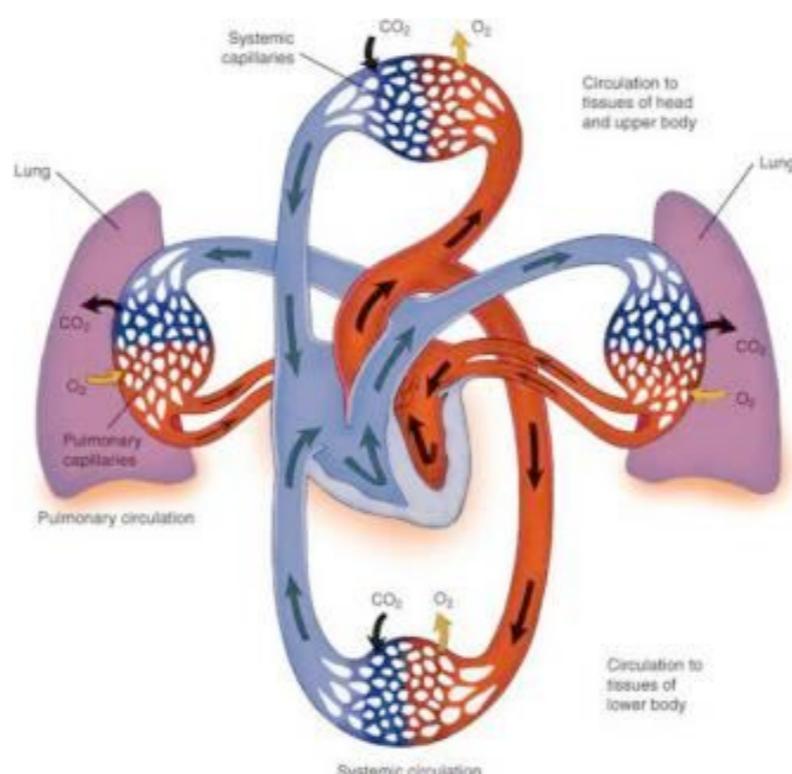
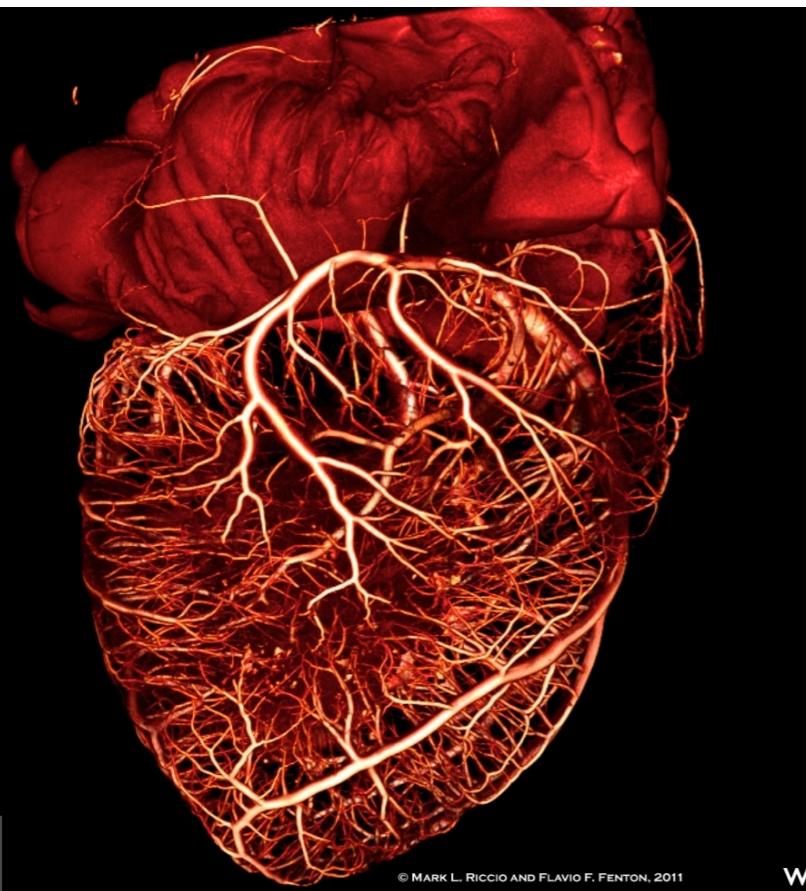
Graph morphometrics

How can one quantify a complex graph?

3d Networks with **restricted** degree?

Vasculature of animal organs, foams etc

n-regular graphs



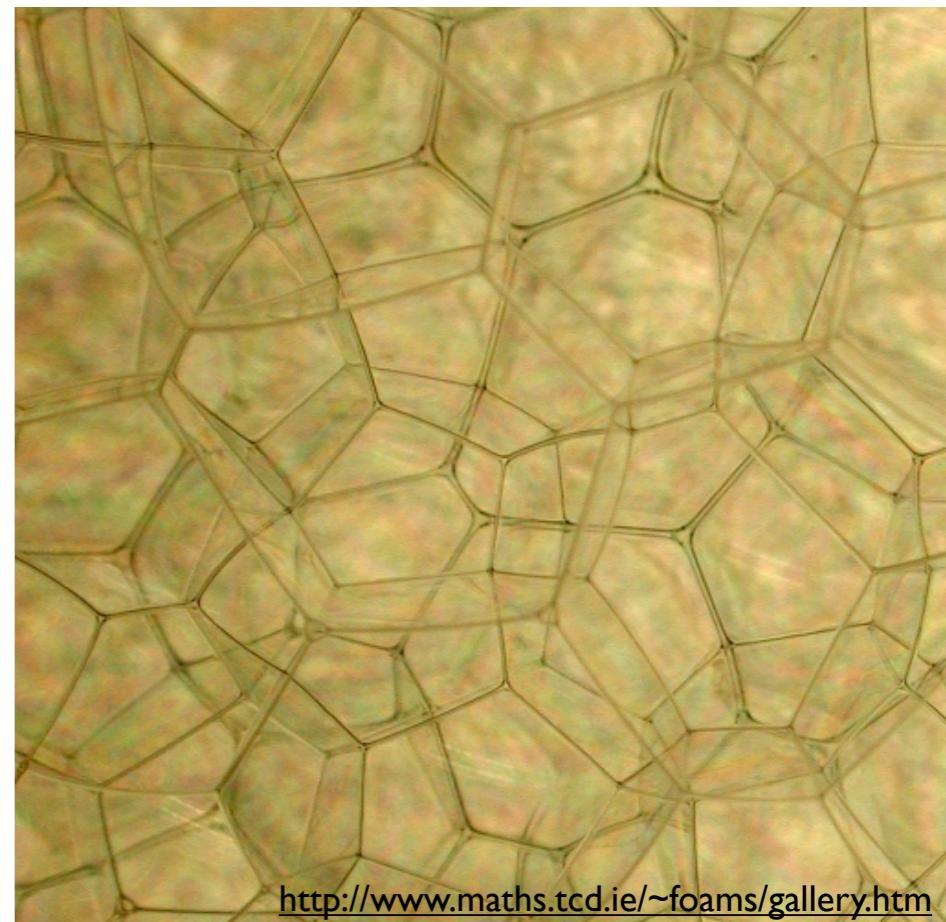
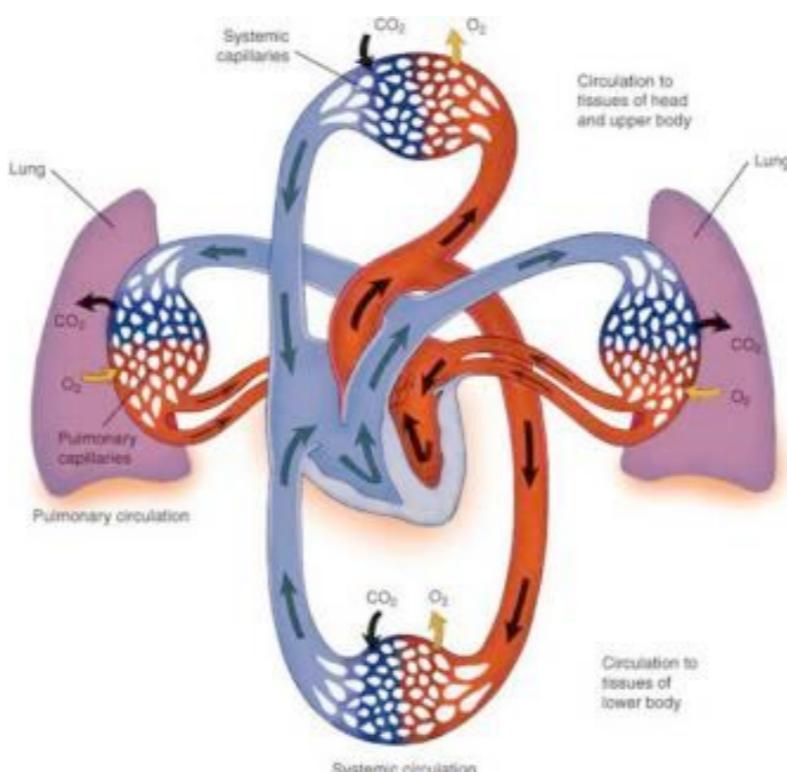
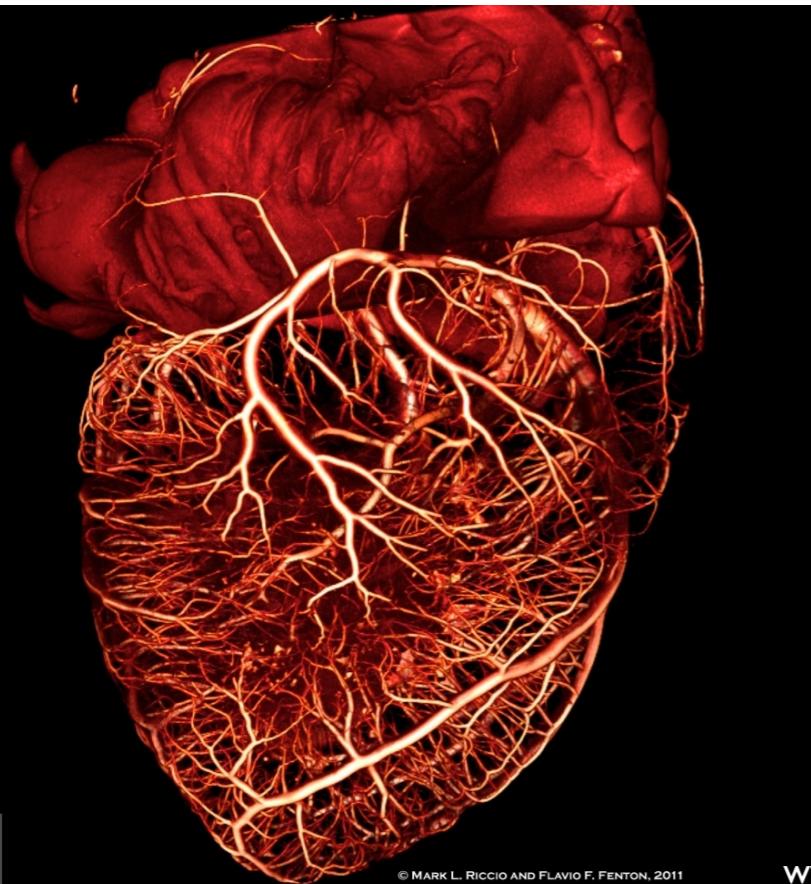
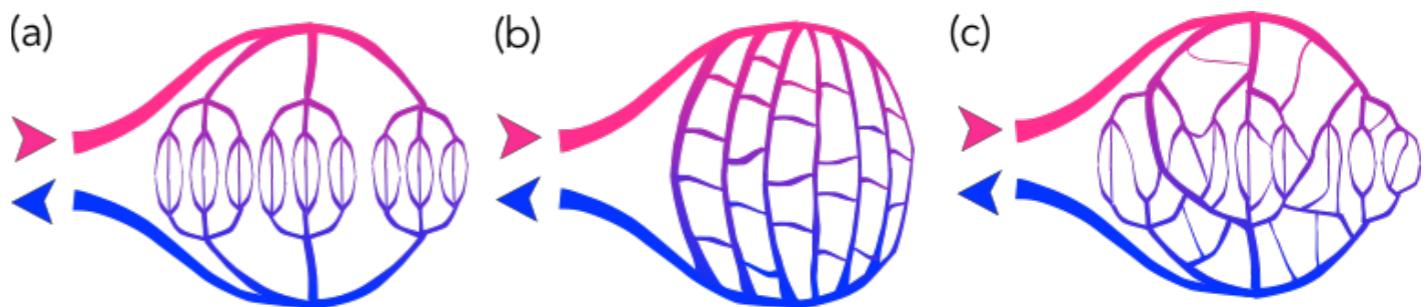
Graph morphometrics

How can one quantify a complex graph?

3d Networks with **restricted** degree?

Vasculature of animal organs, foams etc

n-regular graphs



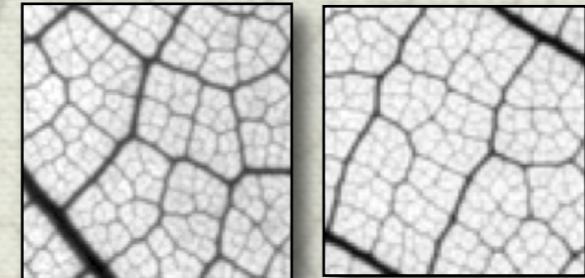
Outline: Quantifying hierarchies in planar graphs

Planar graphs

Motivation

Hierarchical decomposition

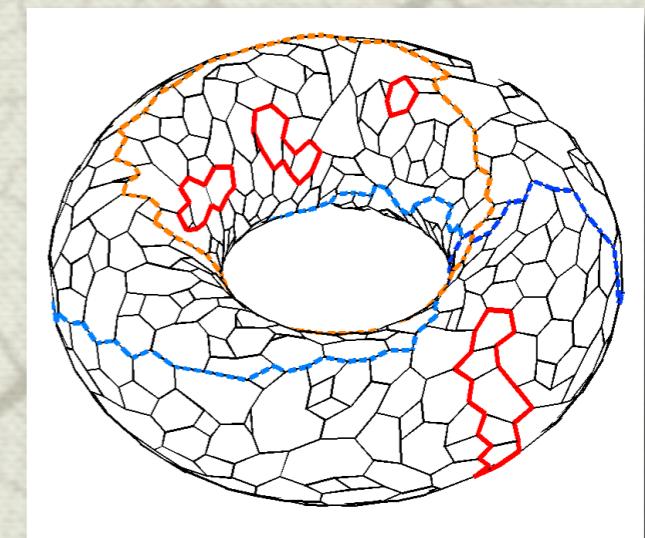
Applications: leaf fingerprinting



Beyond planarity

Every graph can be a planar graph

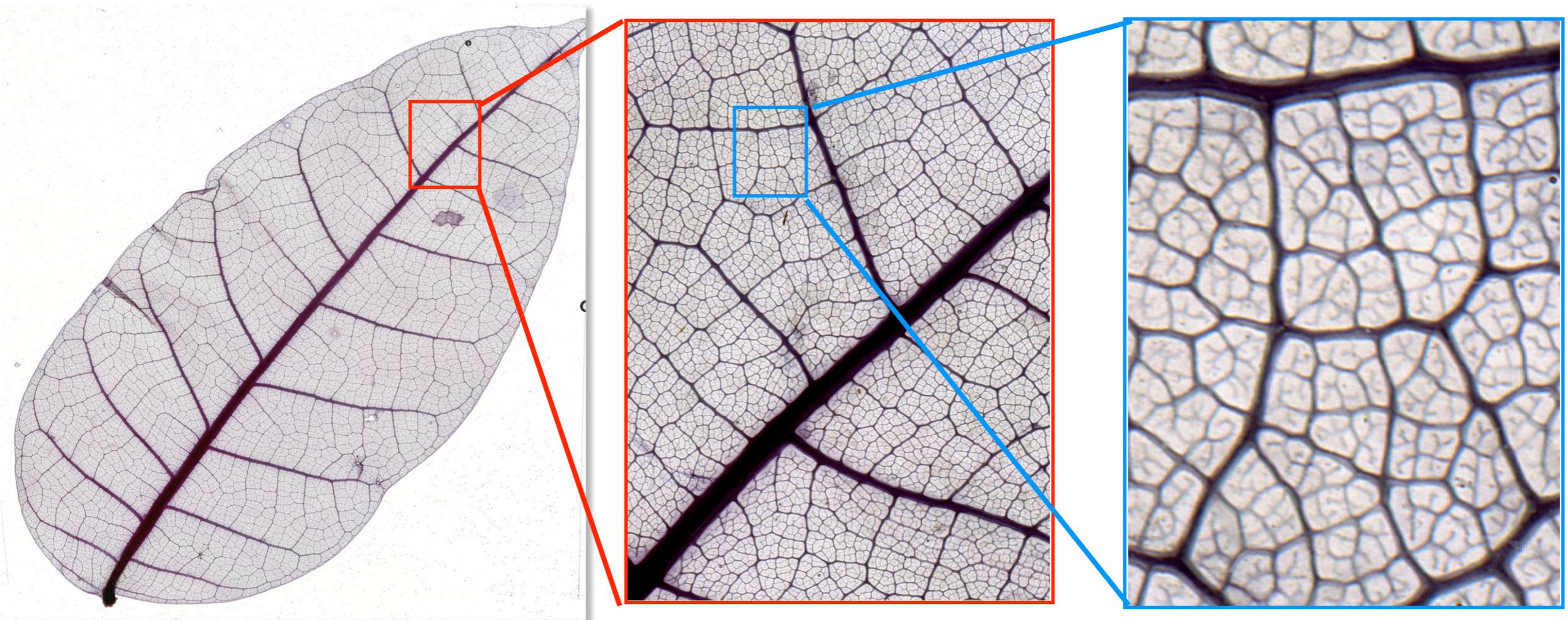
Applications: transportation systems



Leaf vascular architecture: Lots of Loops

Leaves are not trees...

Loops within loops within loops!

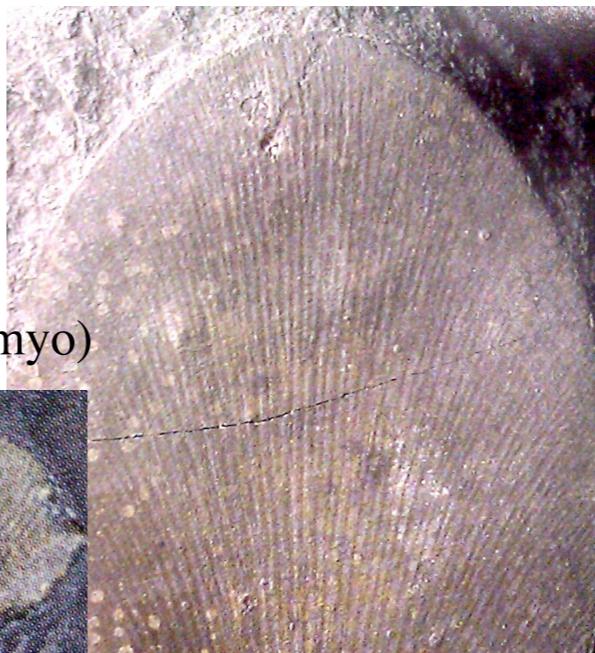
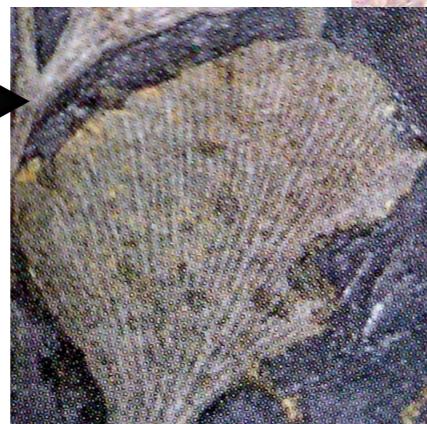


Evolution

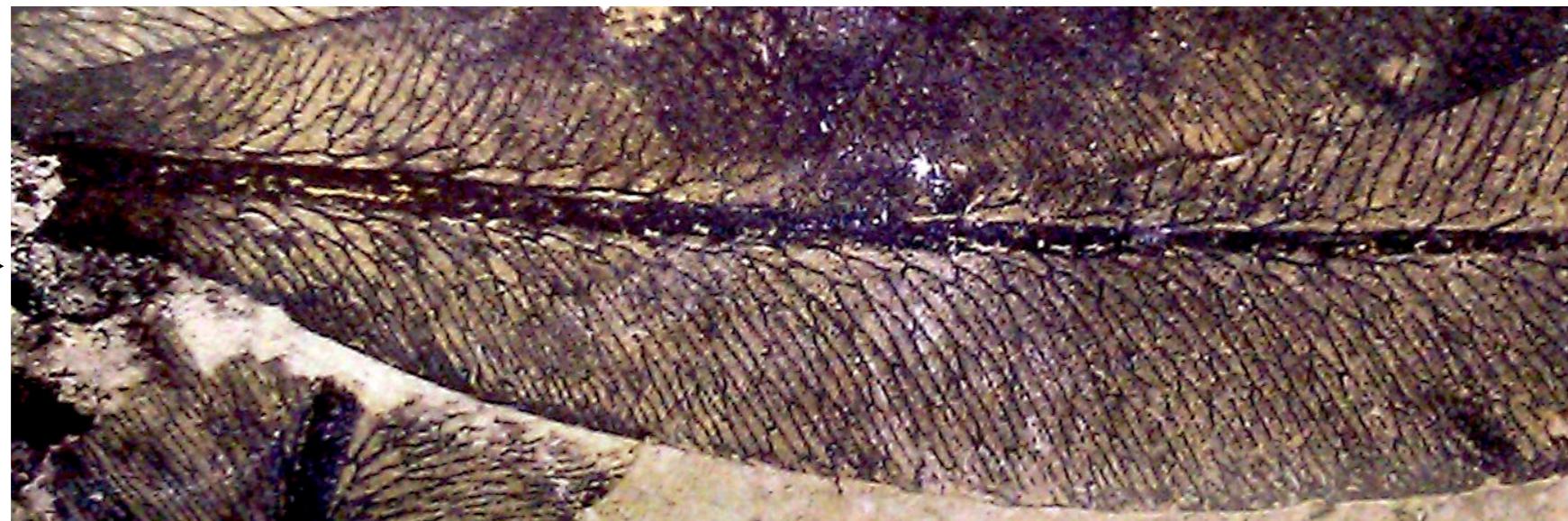


First plants:
dichotomously branching

First leaves:
no loops!
Adiantites (330 myo)

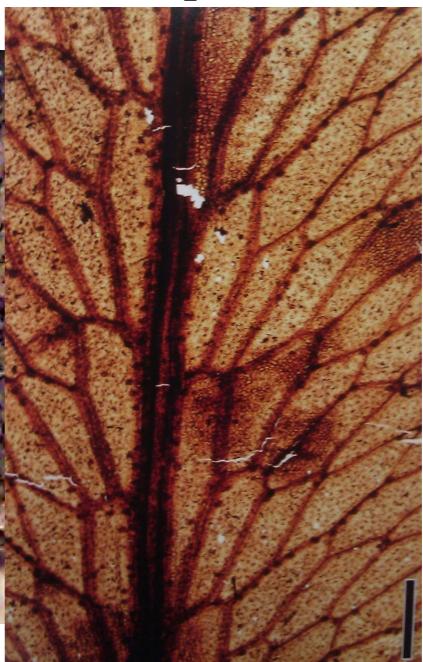


First simple anastomosing patterns



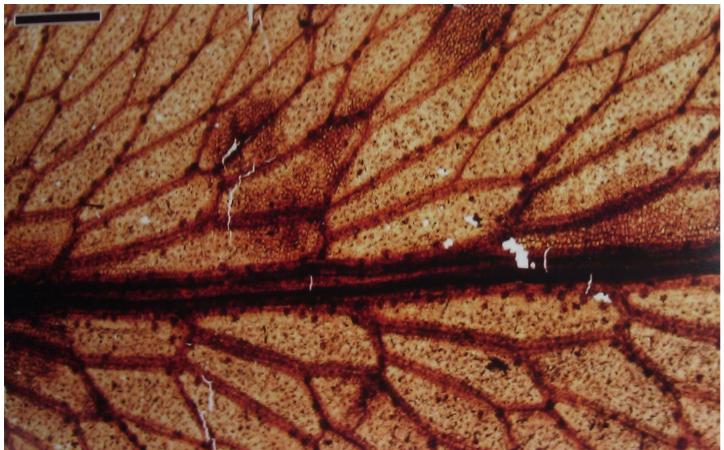
Glossopterys

Barthelopteris (250 myo)



Evolution

Barthelopteris (250 myo)



Evolution of
hierarchical structures



• • •



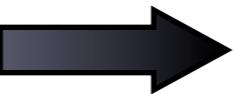
Modern angiosperms

(140 myo)

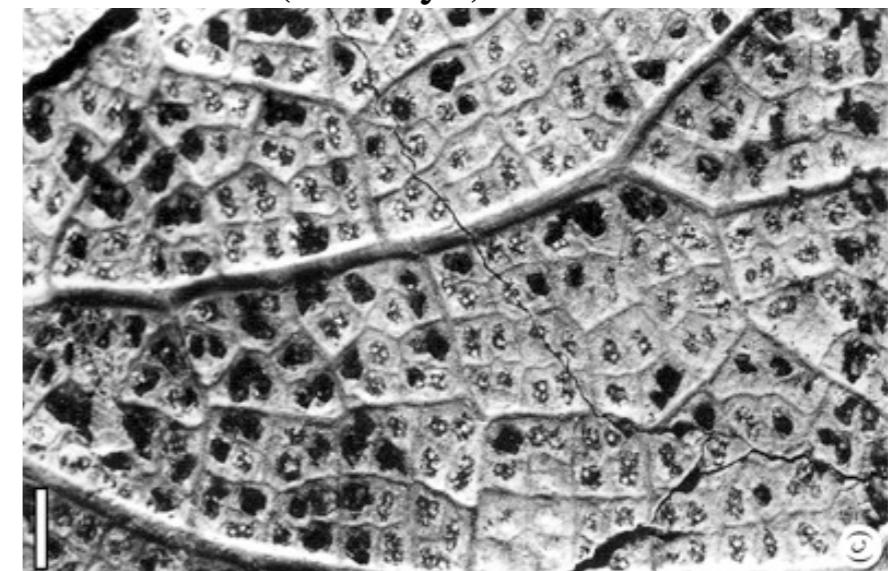


Convergent evolution:

Ferns independently evolved reticulate vascular structures

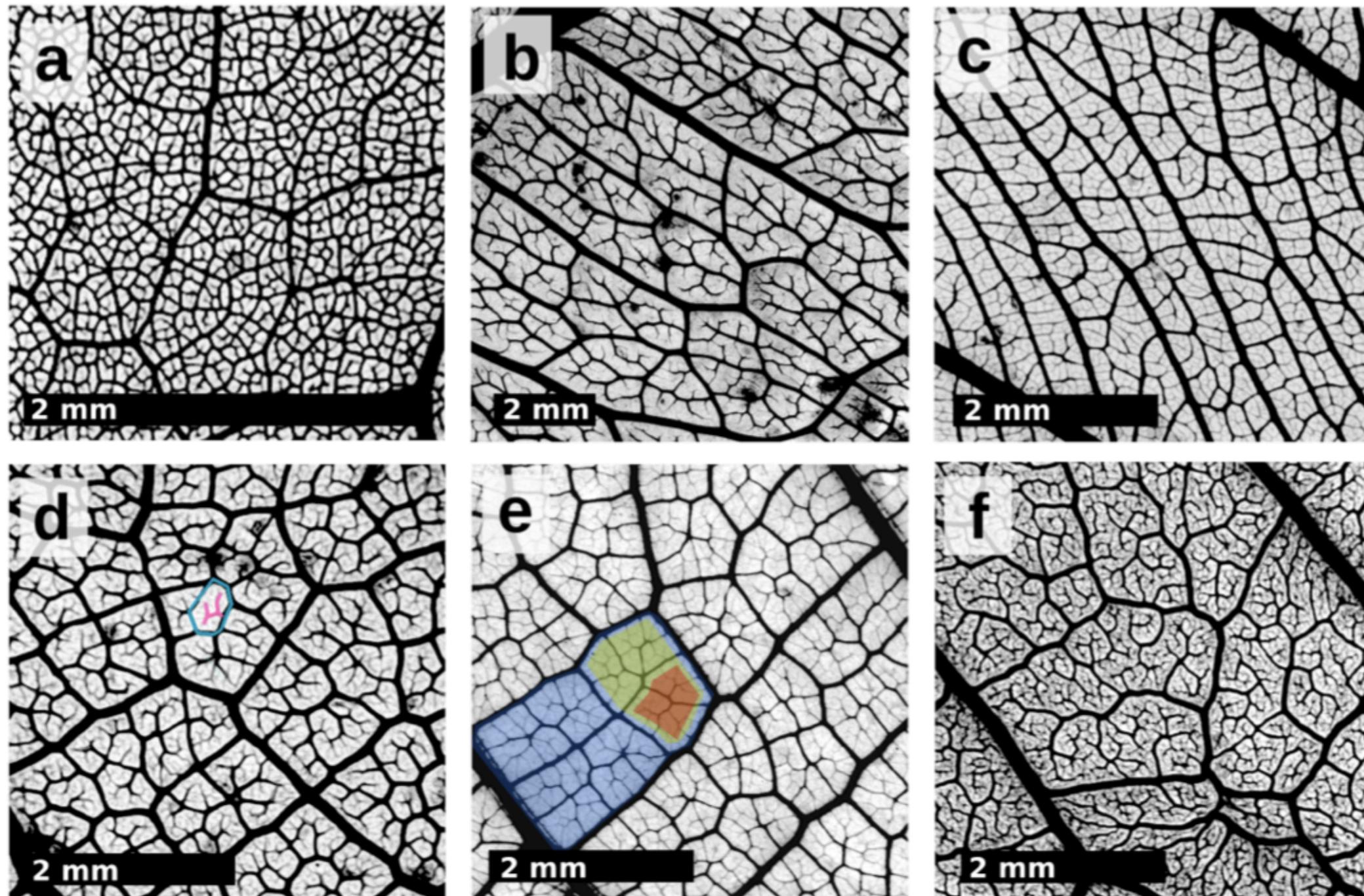


Hausmania (200 myo)



Wang and Zhang (2009)

Quantitative measurement of complex phenotypes



a *Protium ovatum*. b *Protium madagascariense*. c *Pouteria filipes*. d *Canarium betamponae*. A single areole is marked in blue, non-anastomosing highest order veins in red. e *Brosimum guianensis*. The hierarchical nesting of loops is highlighted. f *Protium subserratum*.

Leaf venation phenotypic traits correlate with climate



ARTICLE

Received 23 Mar 2012 | Accepted 10 Apr 2012 | Published 15 May 2012

DOI: 10.1038/ncomms1835

Developmentally based scaling of leaf venation architecture explains global ecological patterns

Lawren Sack¹, Christine Scoffoni¹, Athena D. McKown¹, Kristen Frole², Michael Rawls¹, J. Christopher Havran³, Huy Tran¹ & Thusuong Tran¹



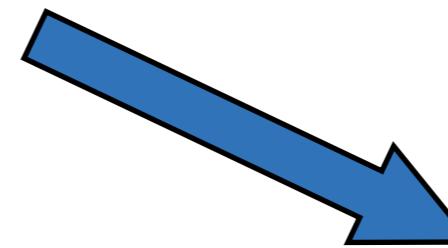
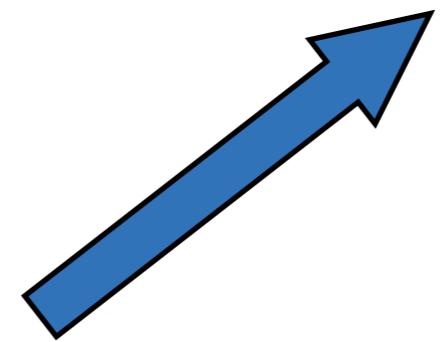
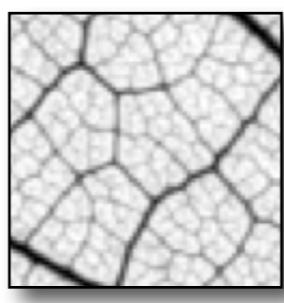
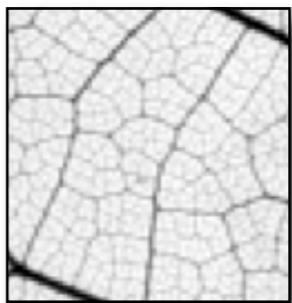
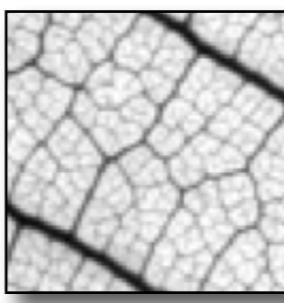
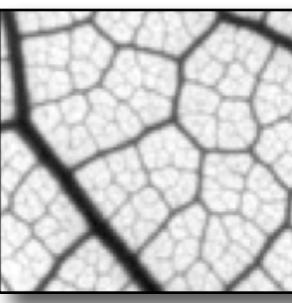
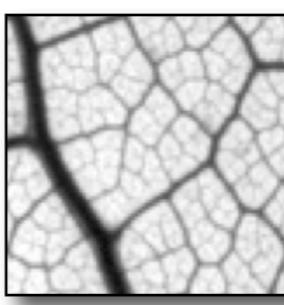
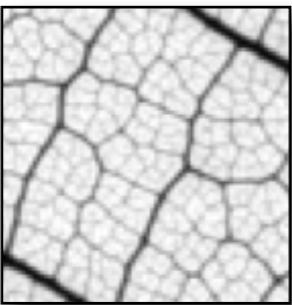
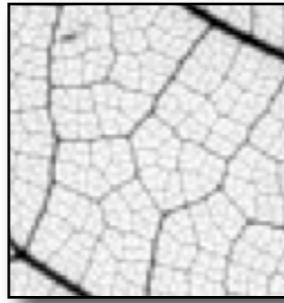
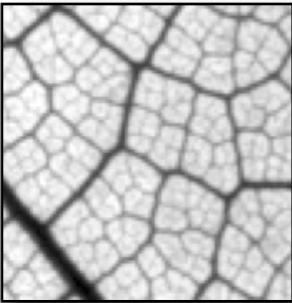
Venation networks and the origin of the leaf economics spectrum

Benjamin Blonder,^{1,*} Cyrille
Violle,^{1,2} Lisa Patrick Bentley¹ and
Brian J. Enquist^{1,3}

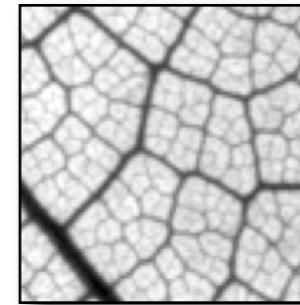
Human venation architecture: implications for disease?

Identification from fragments

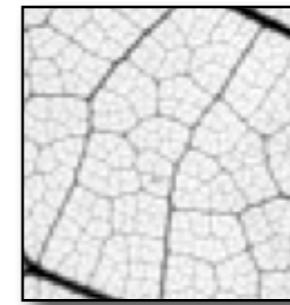
Classify fragments based on feature similarity



Leaf 1

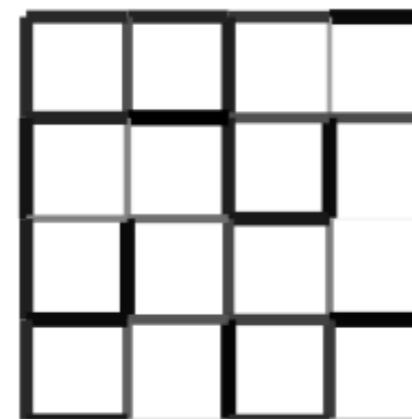
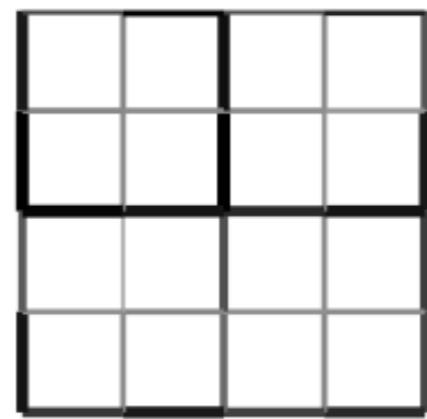
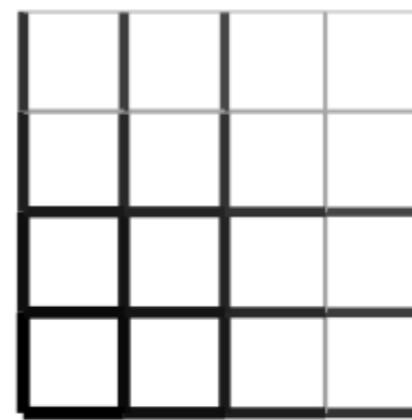
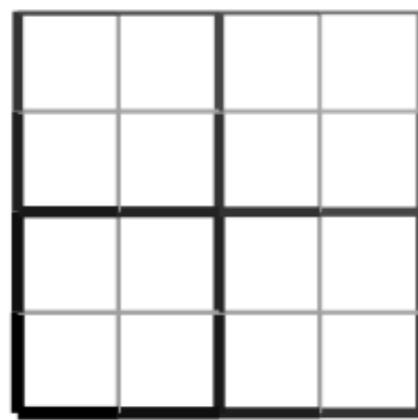


Leaf 2



Identification from fragments

Vein density, vein width distribution, vein density, junction geometry ...
What about connectivity of weighted edges?



Hierarchical decomposition

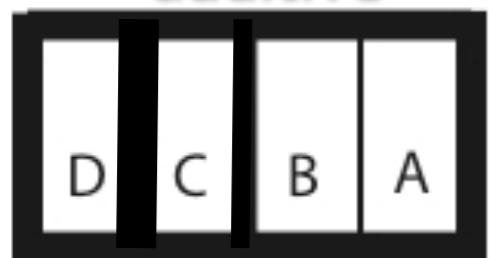
see also
Bohn et al (2005)
Katifori et al (2012)
Mileyko et al (2012)

Hierarchical decomposition

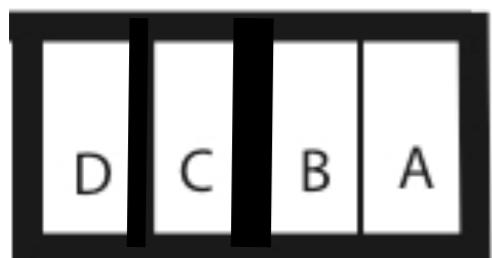
Original network

Building blocks

“additive”



“multiplicative”

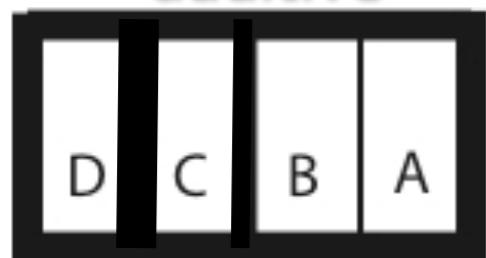


see also
Bohn et al (2005)
Katifori et al (2012)
Mileyko et al (2012)

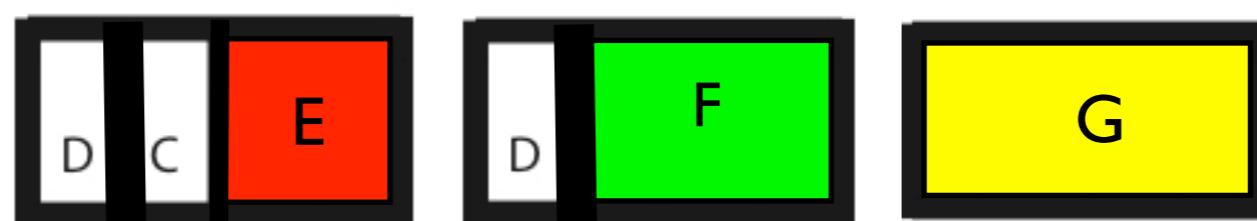
Hierarchical decomposition

Original network

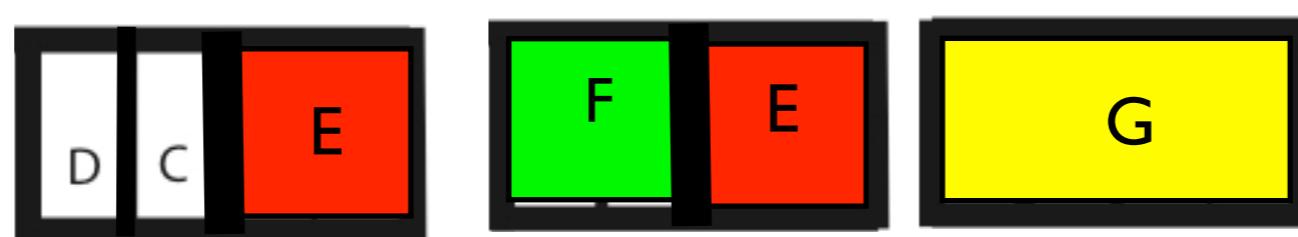
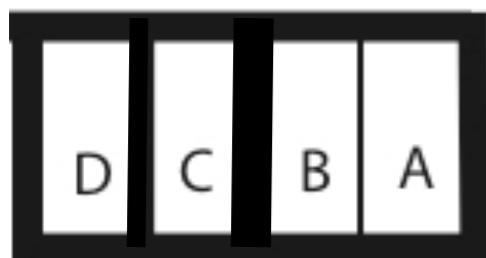
Building blocks
“additive”



Hierarchical decomposition



“multiplicative”

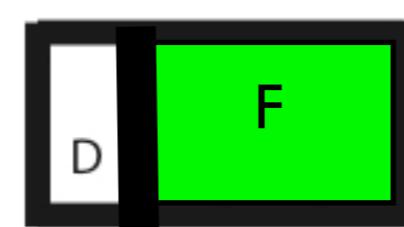
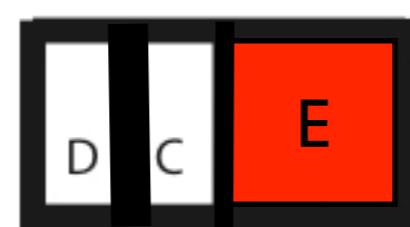
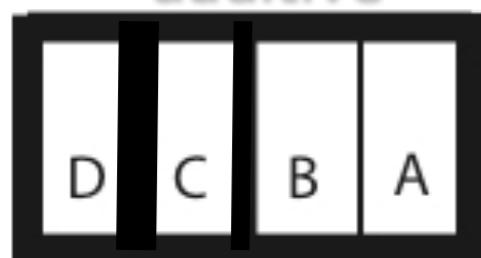


see also
Bohn et al (2005)
Katifori et al (2012)
Mileyko et al (2012)

Hierarchical decomposition

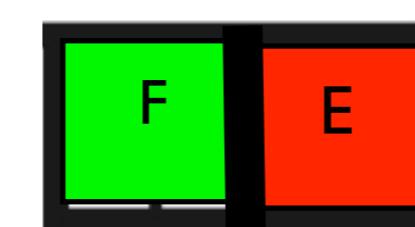
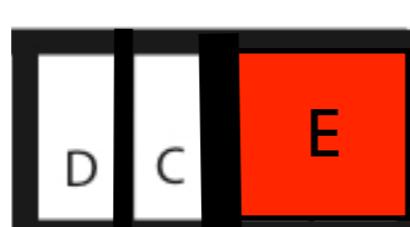
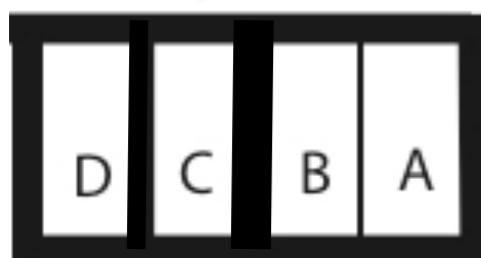
Original network

Building blocks
“additive”

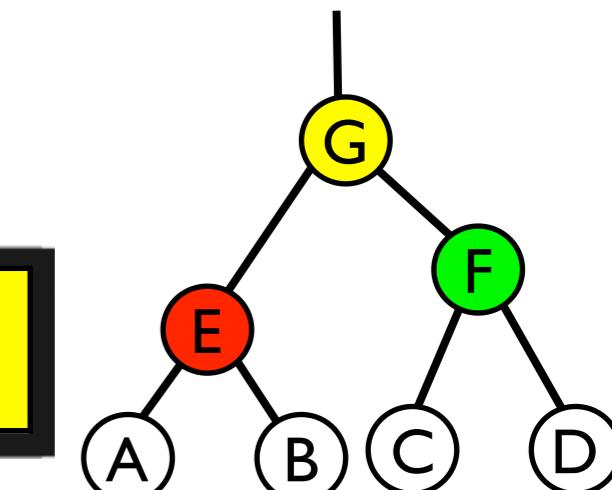
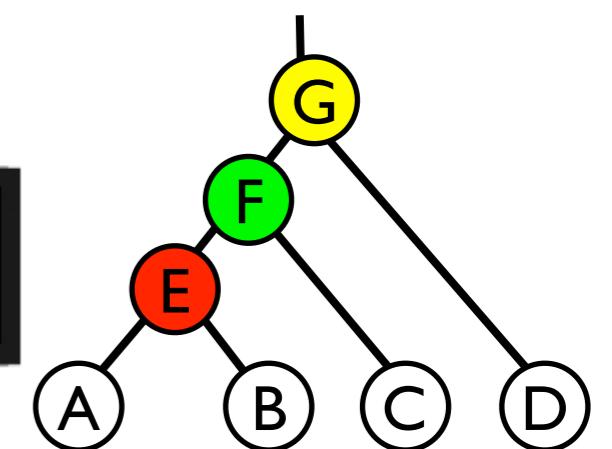


Hierarchical decomposition

“multiplicative”



Nesting tree

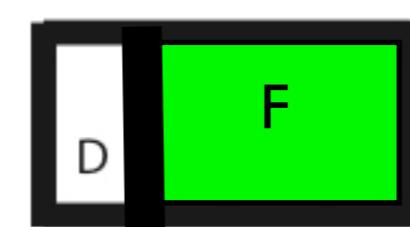
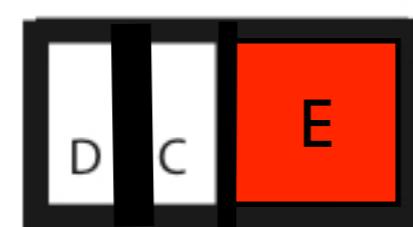
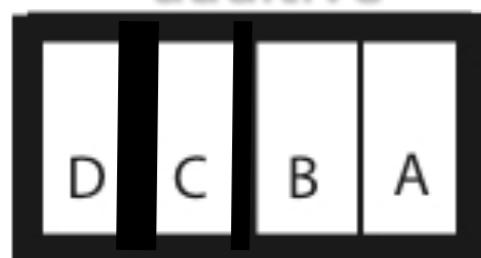


see also
Bohn et al (2005)
Katifori et al (2012)
Mileyko et al (2012)

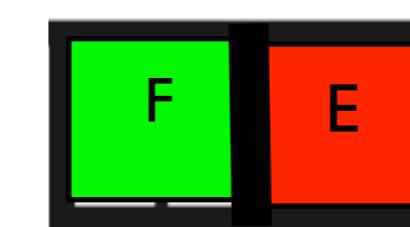
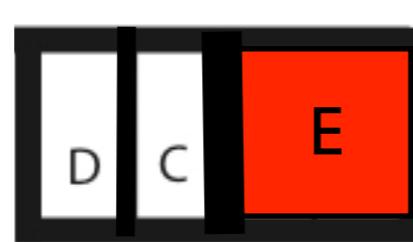
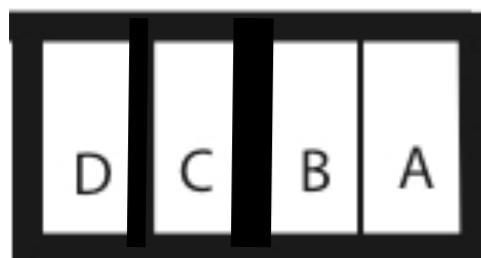
Hierarchical decomposition

Original network

Building blocks
“additive”

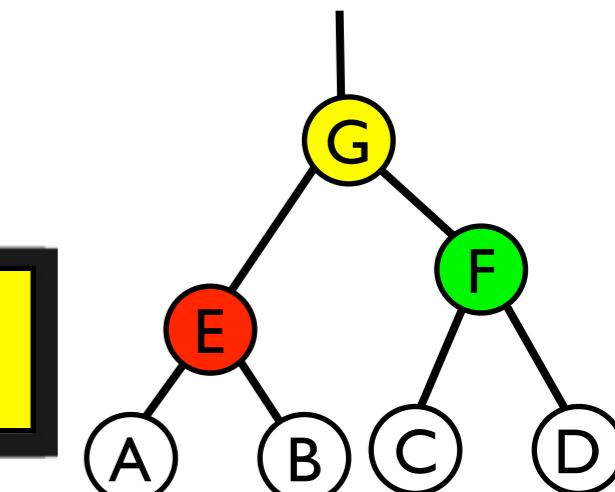
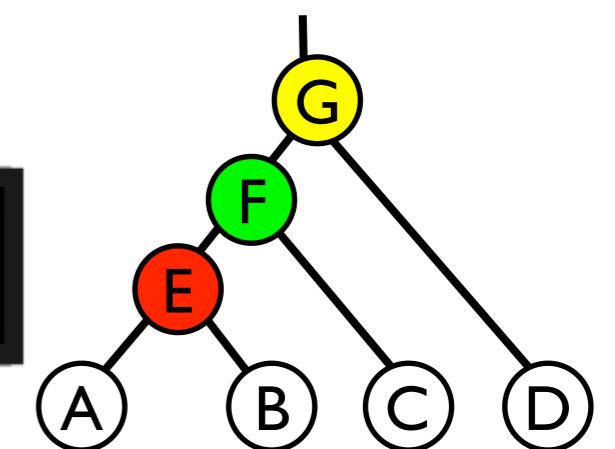


“multiplicative”



Hierarchical decomposition

Nesting tree

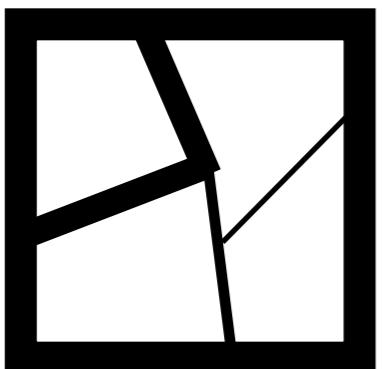


The nesting tree is encoding information about the architecture/topology of the loopy network

see also
Bohn et al (2005)
Katifori et al (2012)
Mileyko et al (2012)

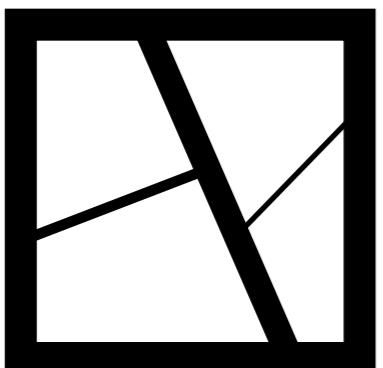
Deciphering the topology

“additive”



gradually subdivided
sequentially adding on same facet

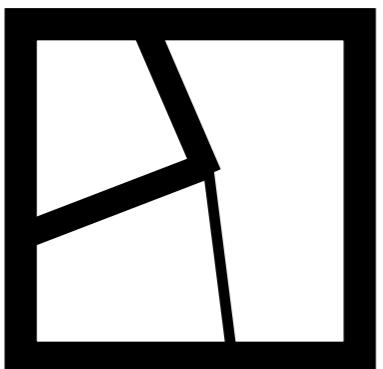
“multiplicative”



aggressively subdivided
different facets growing independently
and then joining

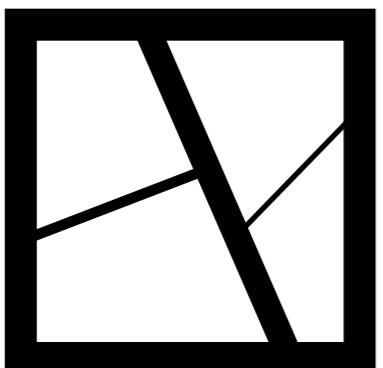
Deciphering the topology

“additive”



gradually subdivided
sequentially adding on same facet

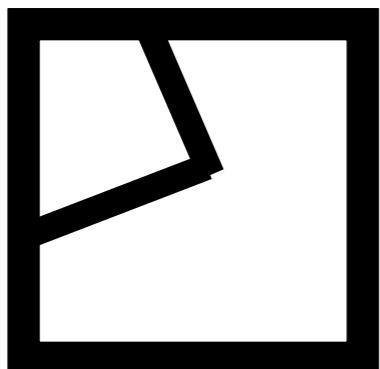
“multiplicative”



aggressively subdivided
different facets growing independently
and then joining

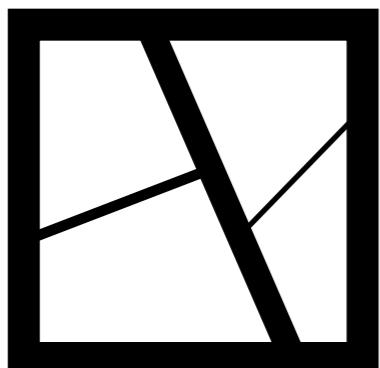
Deciphering the topology

“additive”



gradually subdivided
sequentially adding on same facet

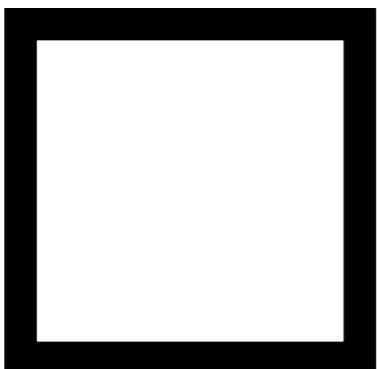
“multiplicative”



aggressively subdivided
different facets growing independently
and then joining

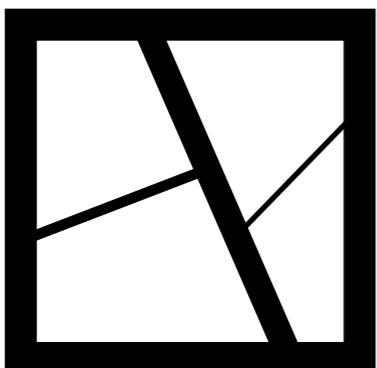
Deciphering the topology

“additive”



gradually subdivided
sequentially adding on same facet

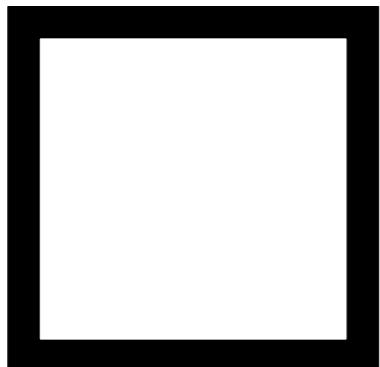
“multiplicative”



aggressively subdivided
different facets growing independently
and then joining

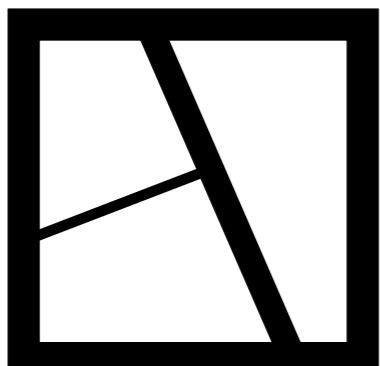
Deciphering the topology

“additive”



gradually subdivided
sequentially adding on same facet

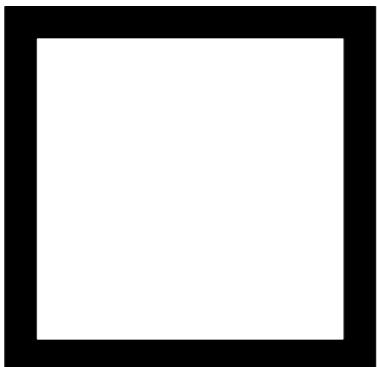
“multiplicative”



aggressively subdivided
different facets growing independently
and then joining

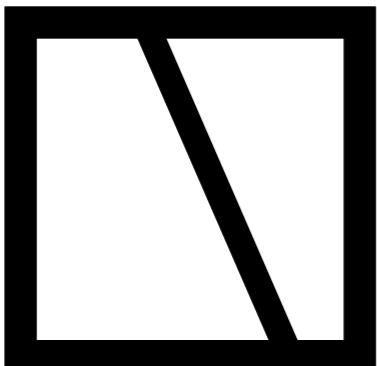
Deciphering the topology

“additive”



gradually subdivided
sequentially adding on same facet

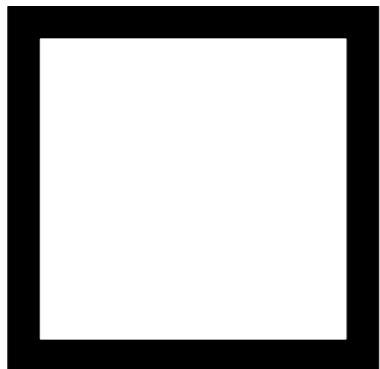
“multiplicative”



aggressively subdivided
different facets growing independently
and then joining

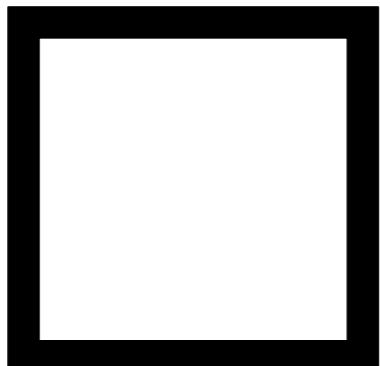
Deciphering the topology

“additive”



gradually subdivided
sequentially adding on same facet

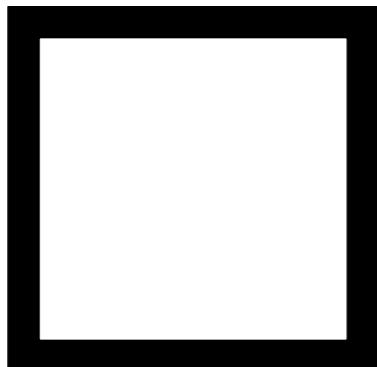
“multiplicative”



aggressively subdivided
different facets growing independently
and then joining

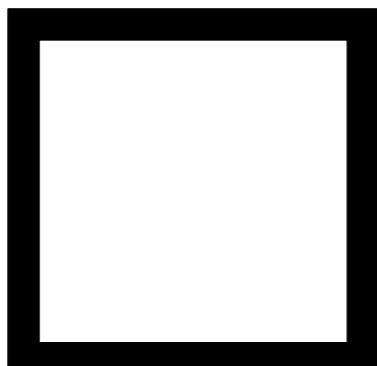
Deciphering the topology

“additive”



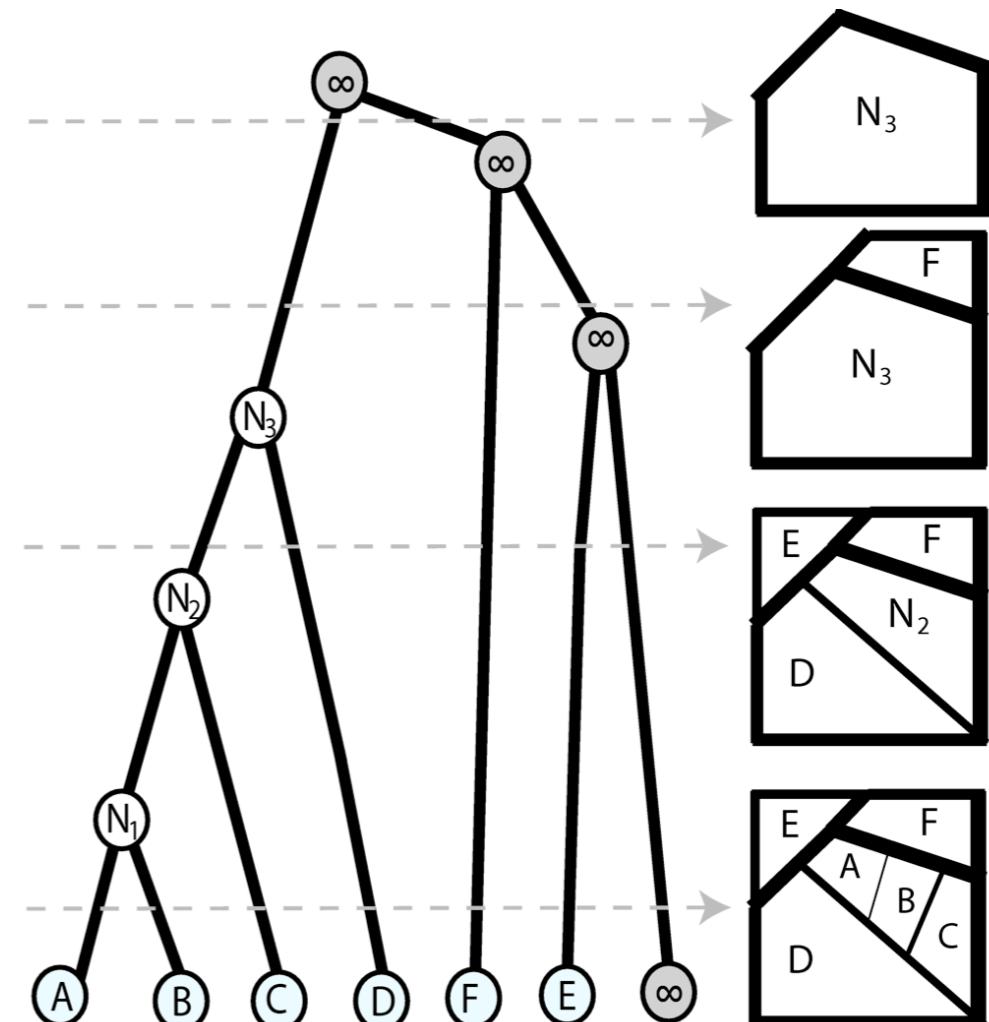
gradually subdivided
sequentially adding on same facet

“multiplicative”



aggressively subdivided
different facets growing independently
and then joining

Hierarchical loopy network decomposition



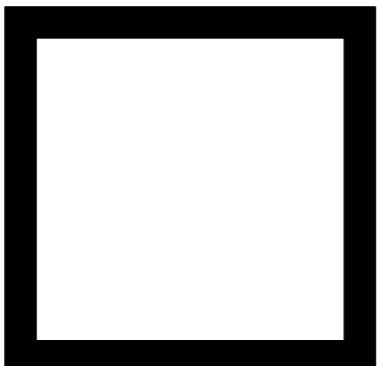
Deciphering the topology

“additive”



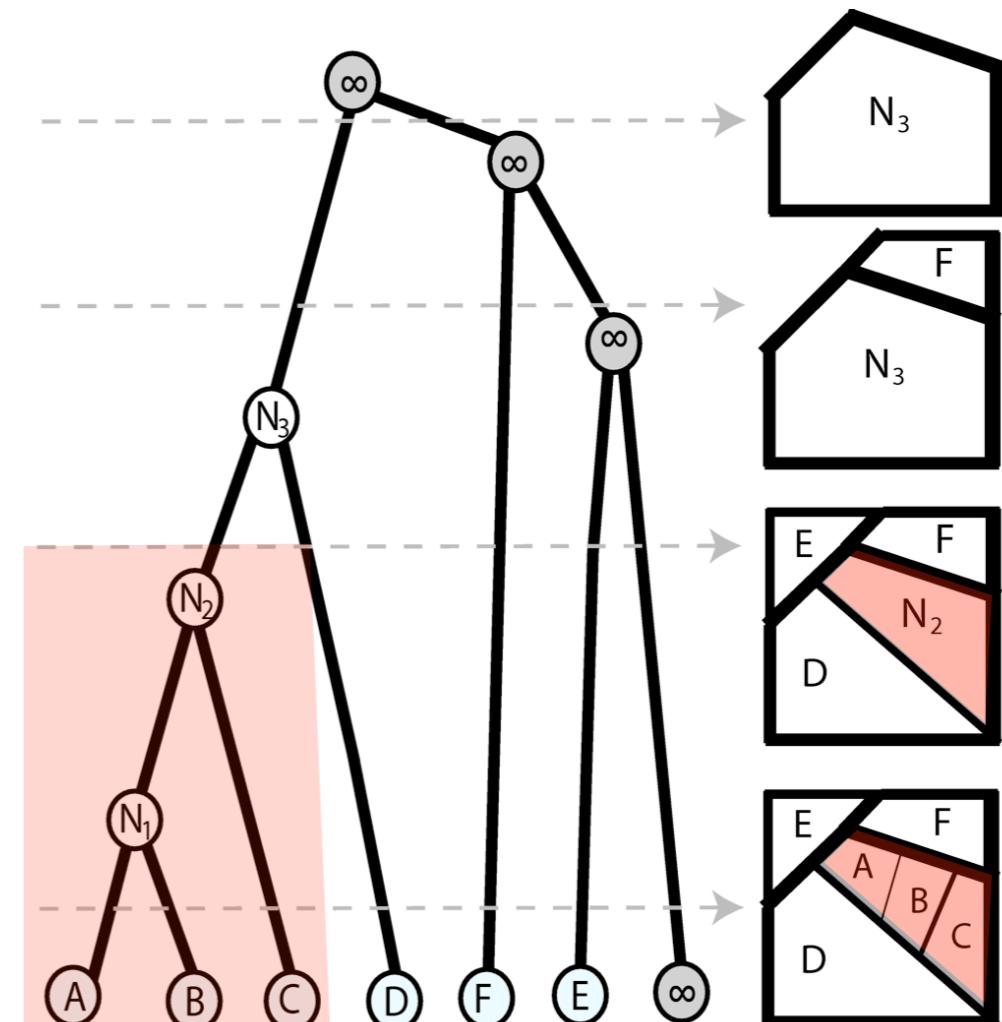
gradually subdivided
sequentially adding on same facet

“multiplicative”



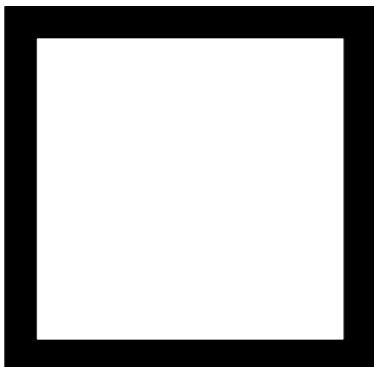
aggressively subdivided
different facets growing independently
and then joining

Hierarchical loopy network decomposition



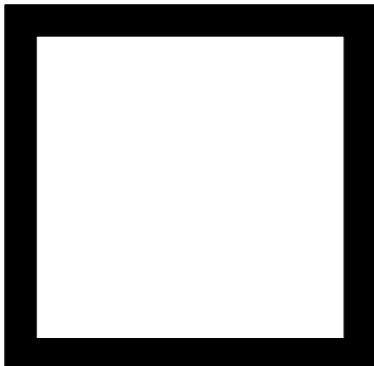
Deciphering the topology

“additive”



gradually subdivided
sequentially adding on same facet

“multiplicative”



aggressively subdivided
different facets growing independently
and then joining

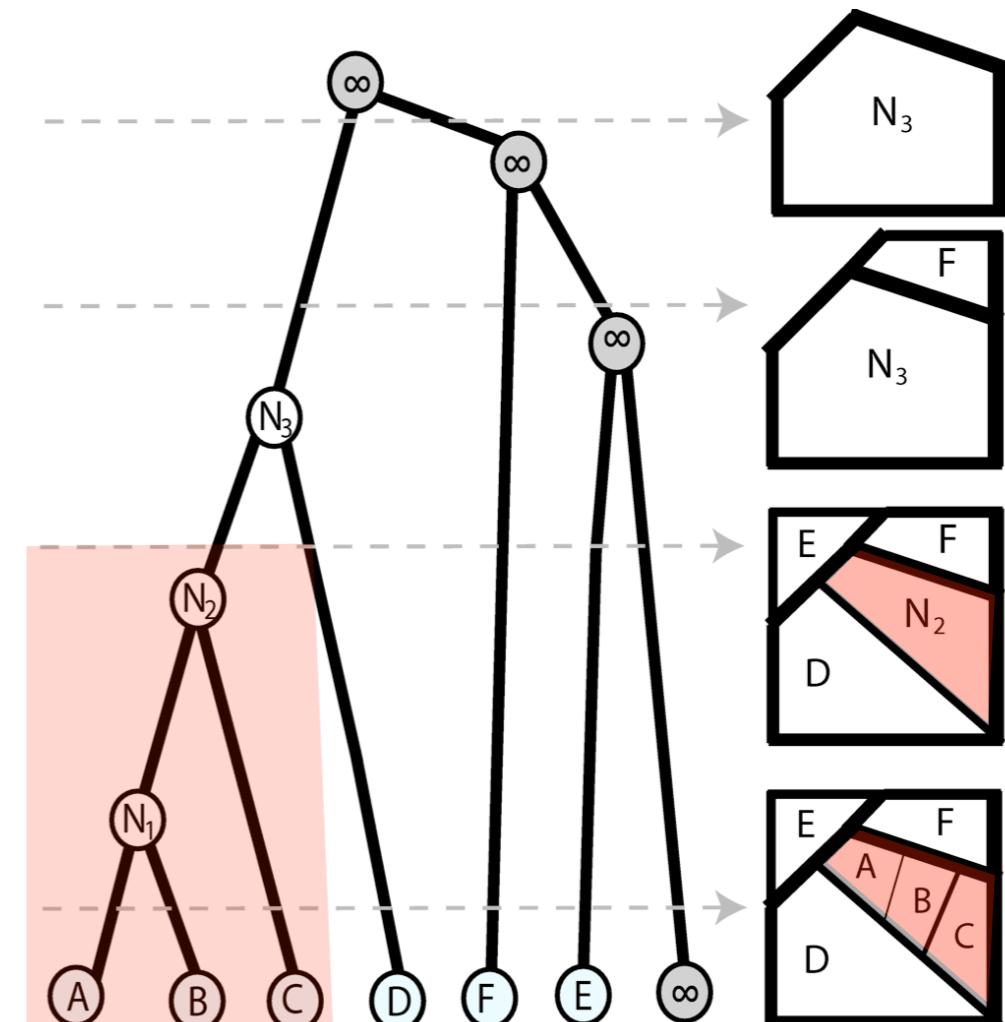
filtration

$b_1 = 3$

$b_1 = 5$

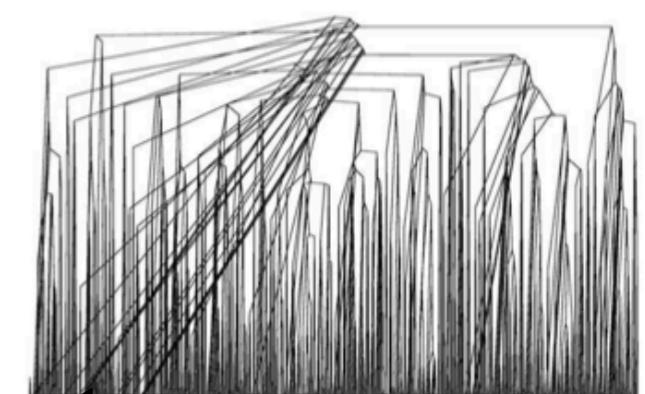
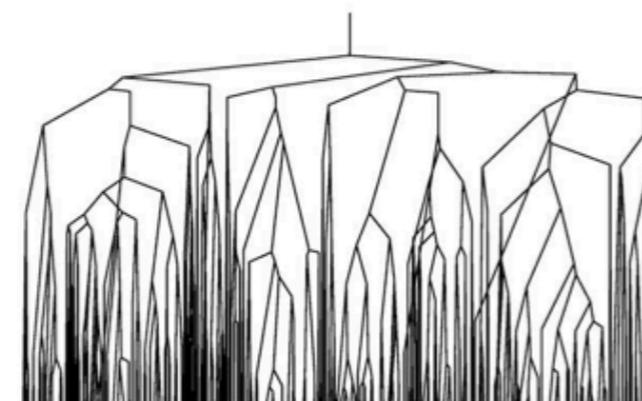
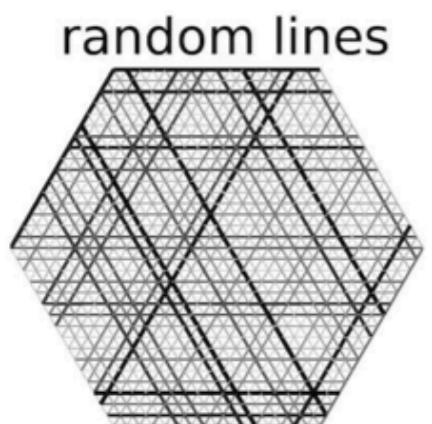
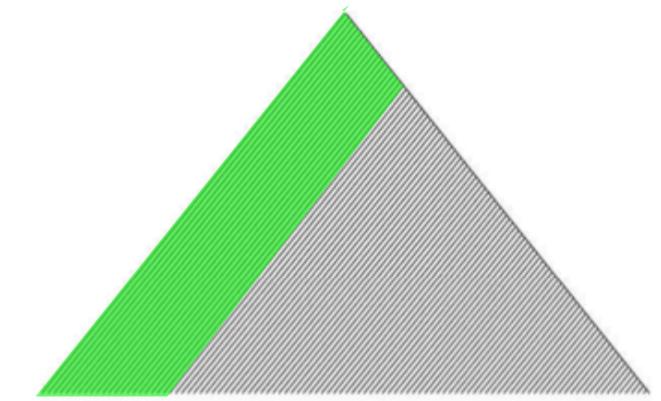
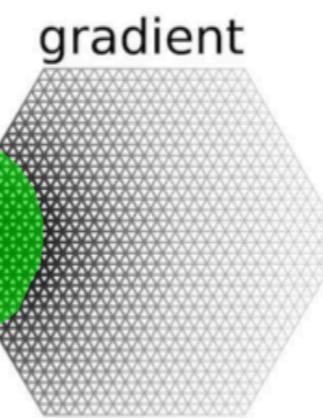
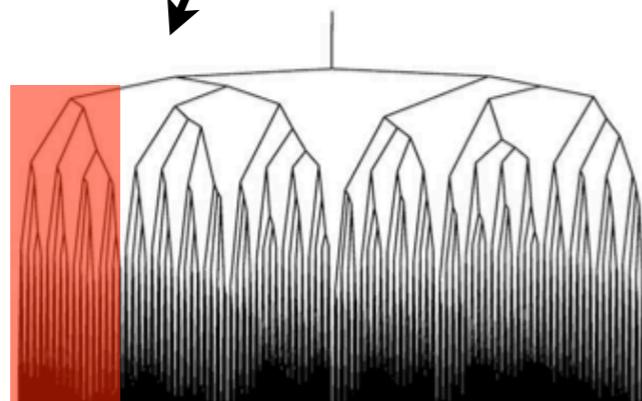
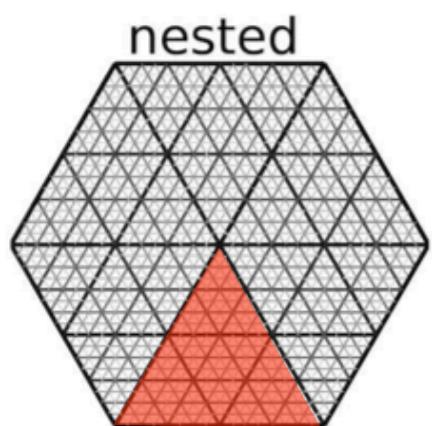
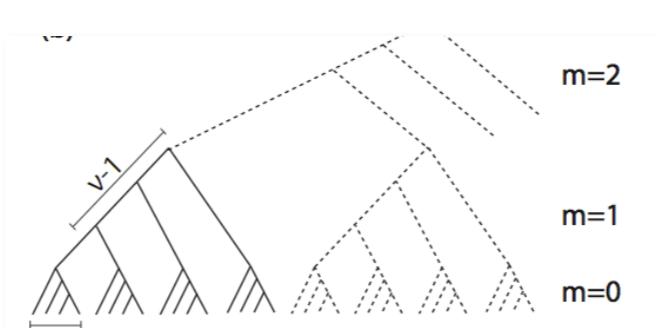
$b_1 = 7$

Hierarchical loopy network decomposition



Deciphering the topology

Assess fractal nature of topological organization



Deciphering the topology

Asymmetry

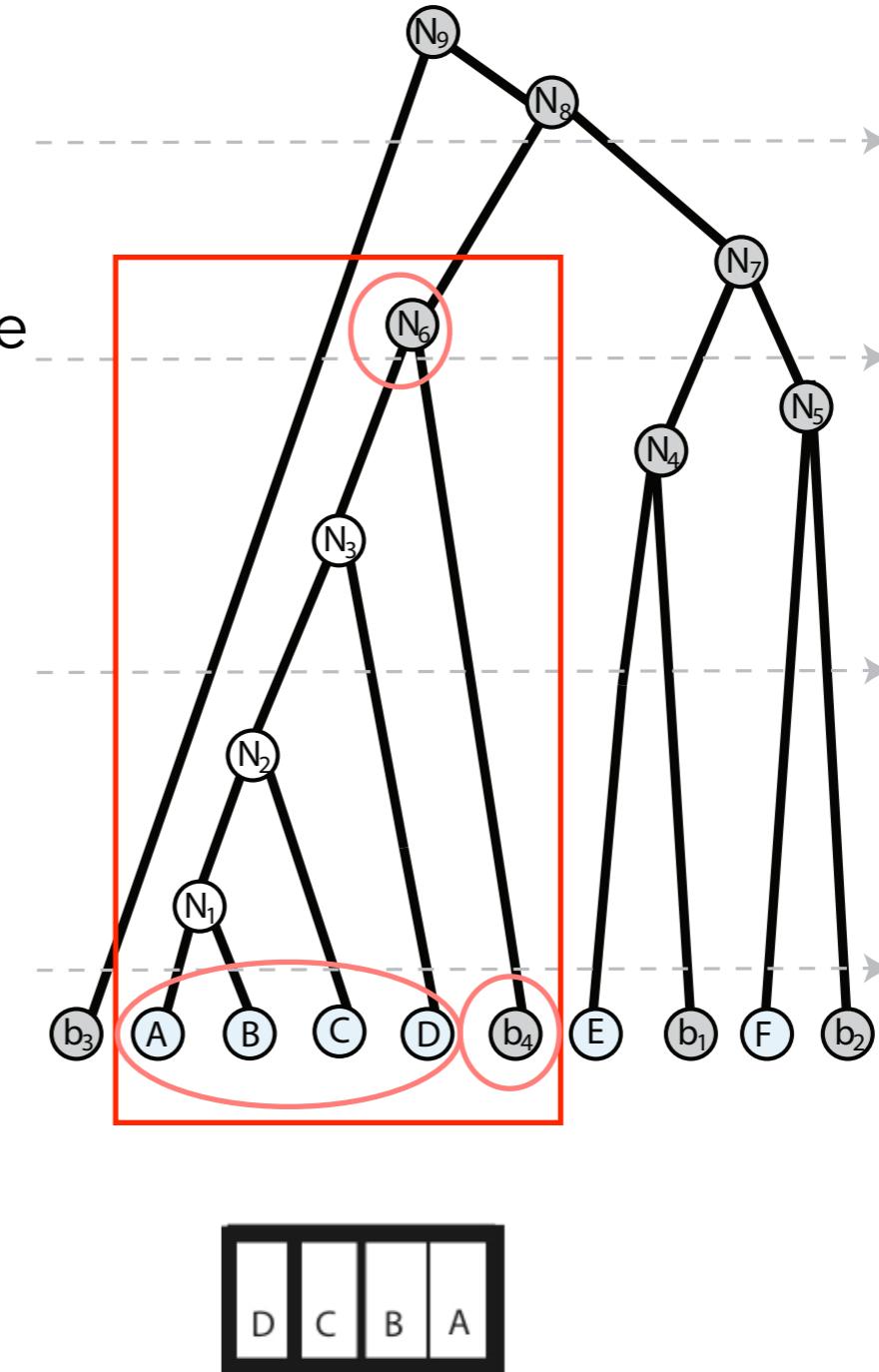
Assigns a number to each node of the tree based on the similarity of the two joining subtrees

Van Pelt et al (1992)

$$q(r_j, s_j) = \frac{s_j - r_j}{s_j}$$

$$Q_T(t_n) = \frac{1}{w(t_n)} \sum_{j=1}^{d(n)-1} w_j q(r_j, s_j)$$

$$w(t_n) = \sum_{j=1}^{d(n)-1} w_j.$$



Deciphering the topology

Asymmetry

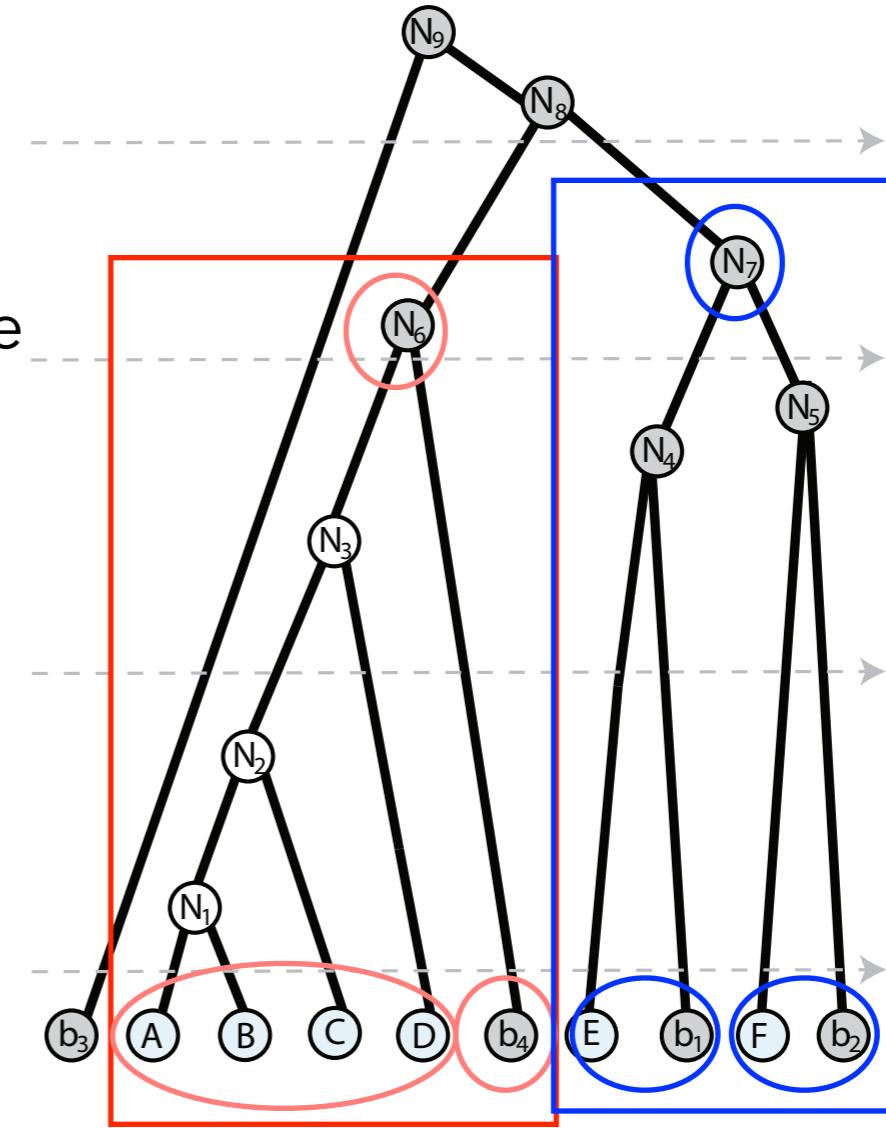
Assigns a number to each node of the tree based on the similarity of the two joining subtrees

Van Pelt et al (1992)

$$q(r_j, s_j) = \frac{s_j - r_j}{s_j}$$

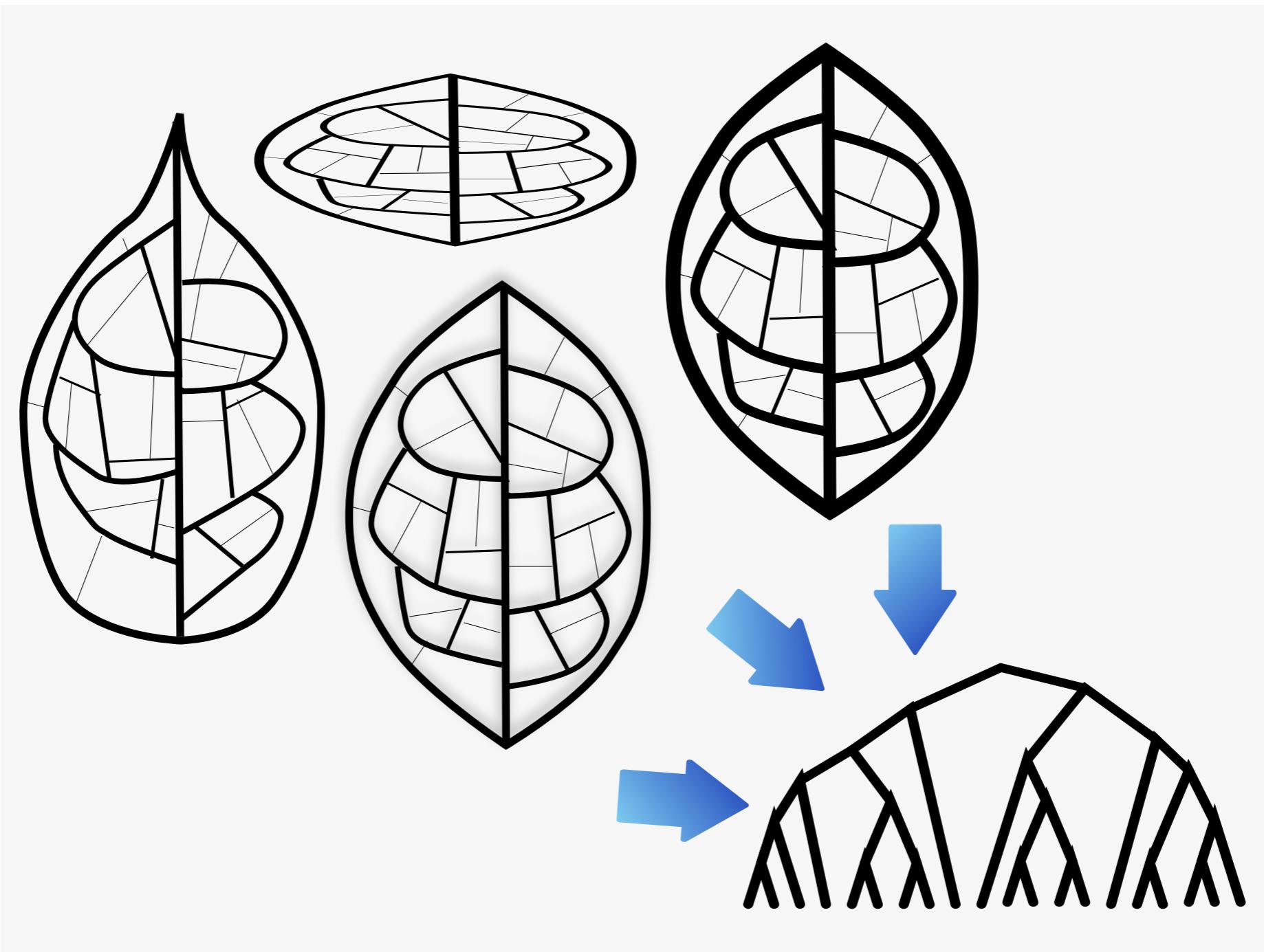
$$Q_T(t_n) = \frac{1}{w(t_n)} \sum_{j=1}^{d(n)-1} w_j q(r_j, s_j)$$

$$w(t_n) = \sum_{j=1}^{d(n)-1} w_j.$$

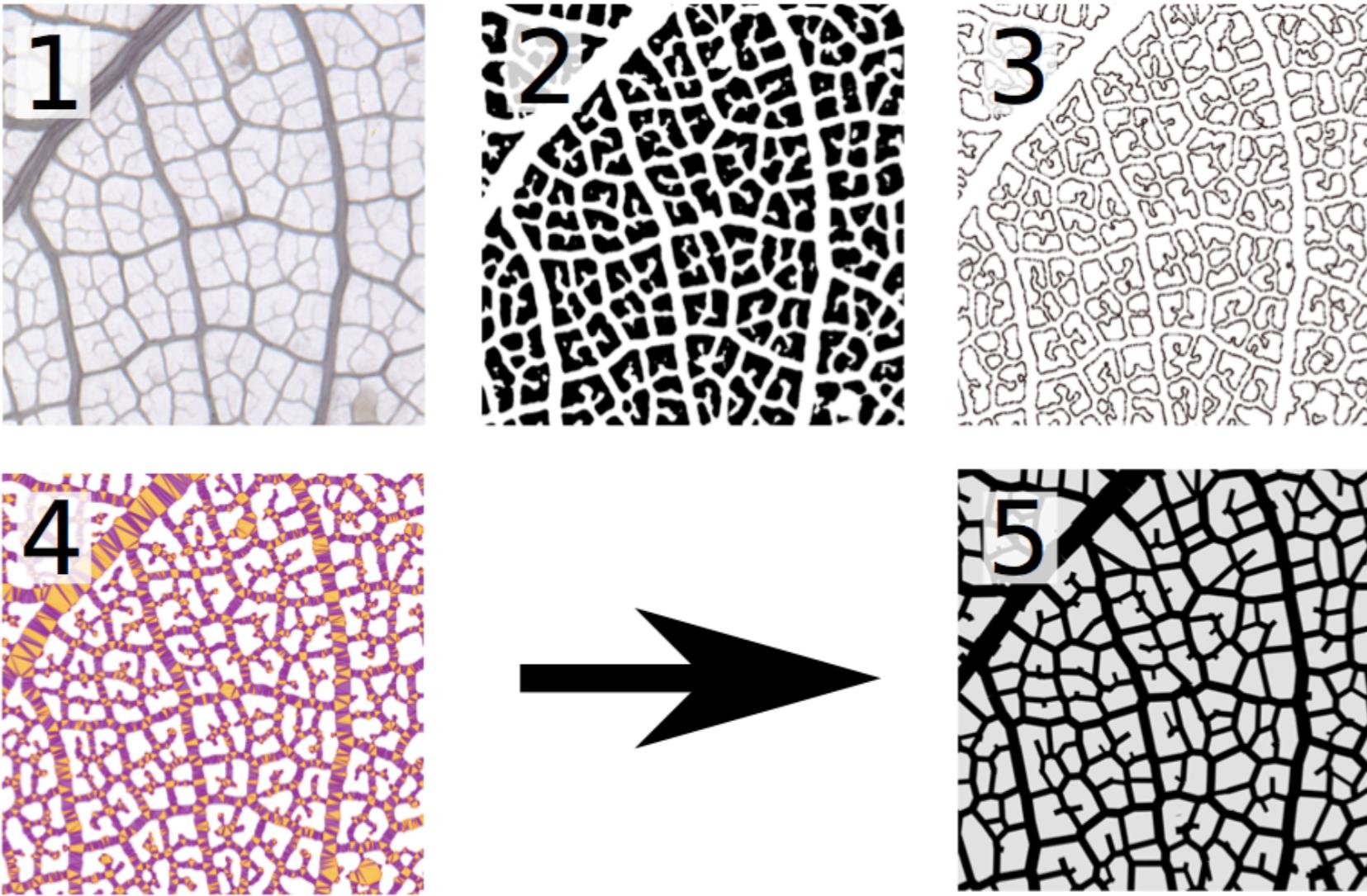


Deciphering the topology

Information about geometry and weight is decoupled
only topology and sort order of edges matters



Leaf fingerprinting

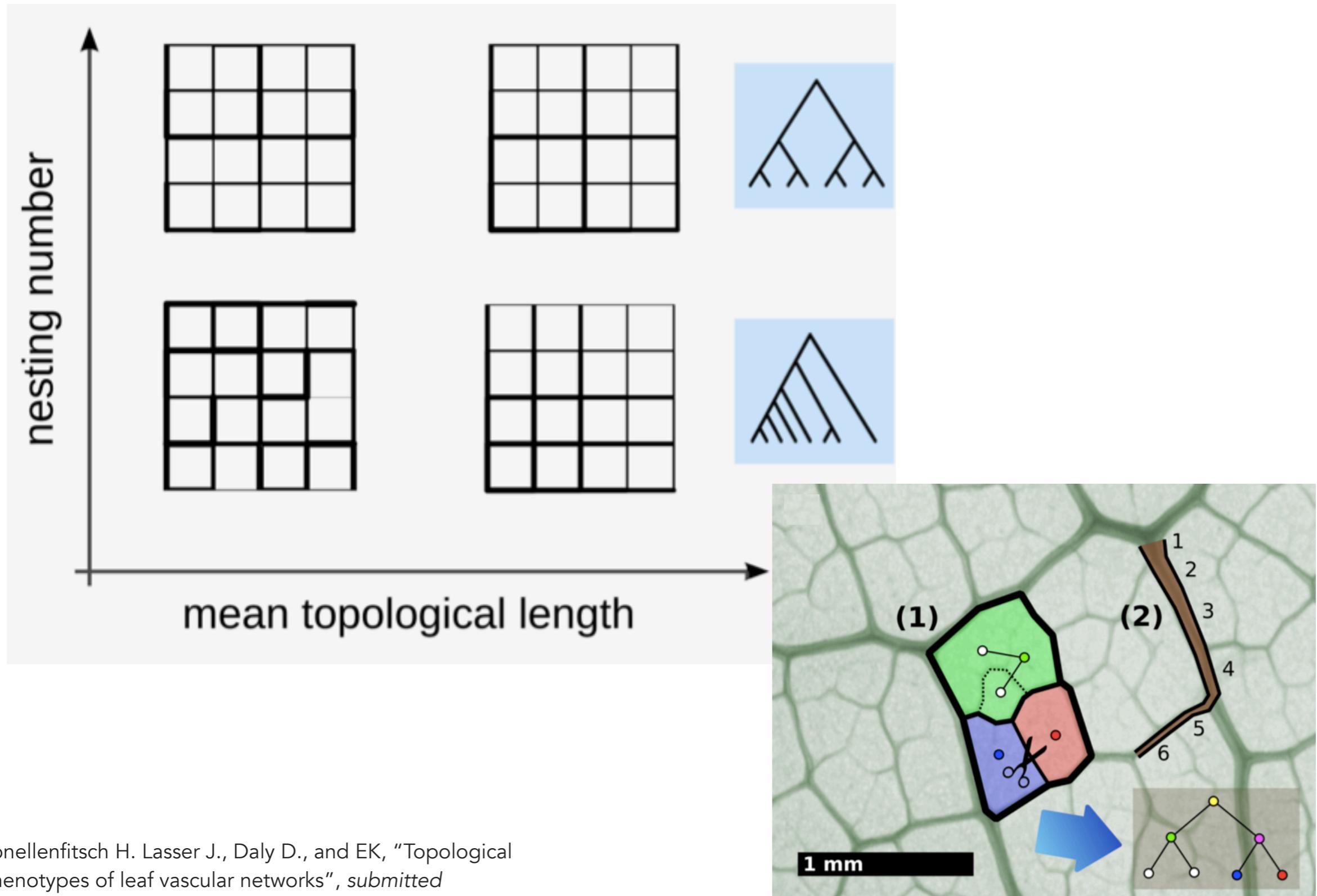


The vectorization process.

(1) start from a high resolution scanned image (6400 dpi) (2) binarize using a combination of blurring, local histogram equalization and finally Otsu thresholding. (3) Teh- Chin dominant point detection to obtain a set of contour points. (4) Constrained Delaunay triangulation of the contour points. (5) The final graph representation of the vascular network.

Leaf fingerprinting

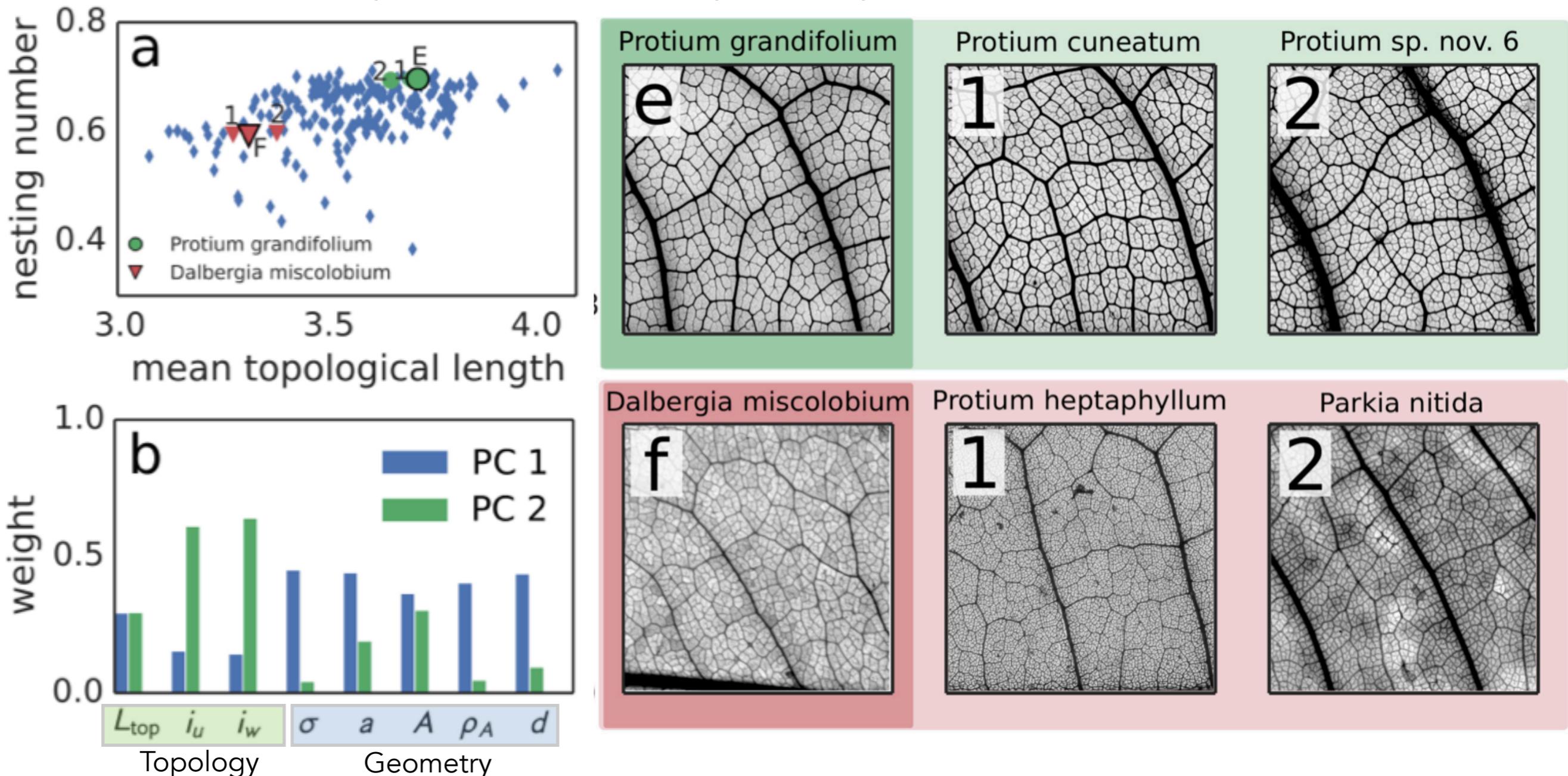
Topological phenotypes



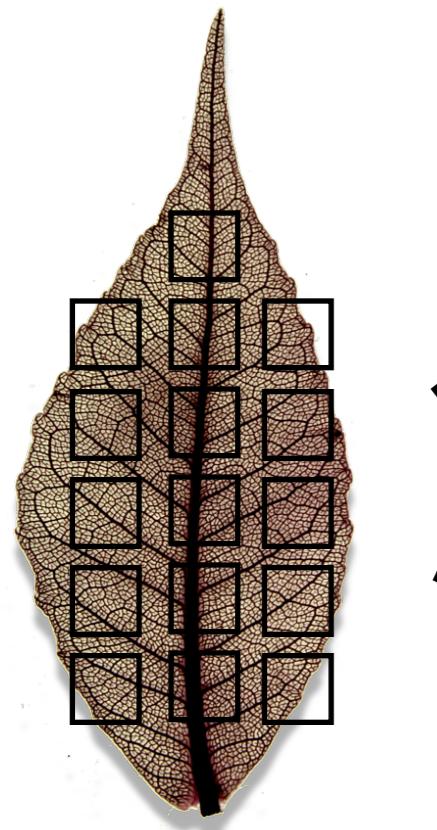
Leaf fingerprinting

Geometry carries information orthogonal to topology

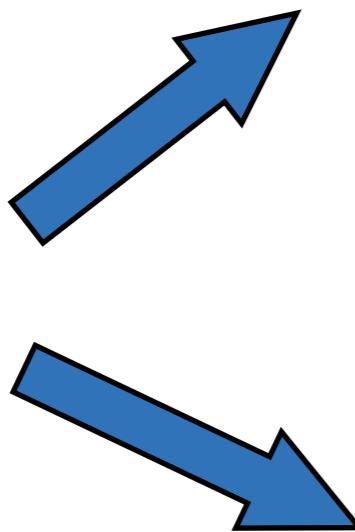
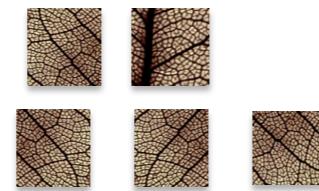
Geometry and topology are distinct phenotypes



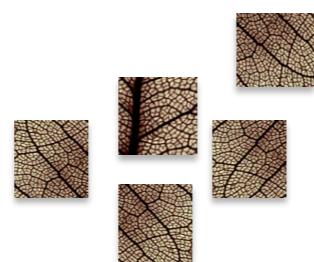
Leaf fingerprinting



training set



test set



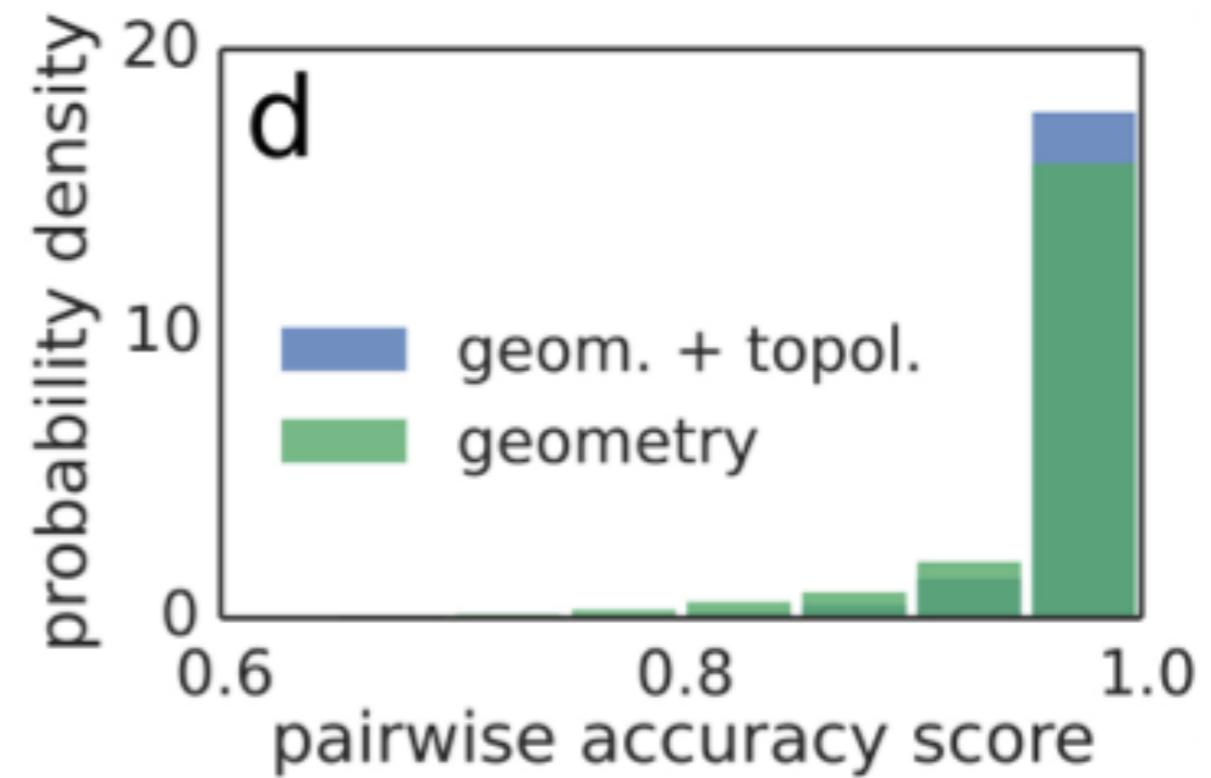
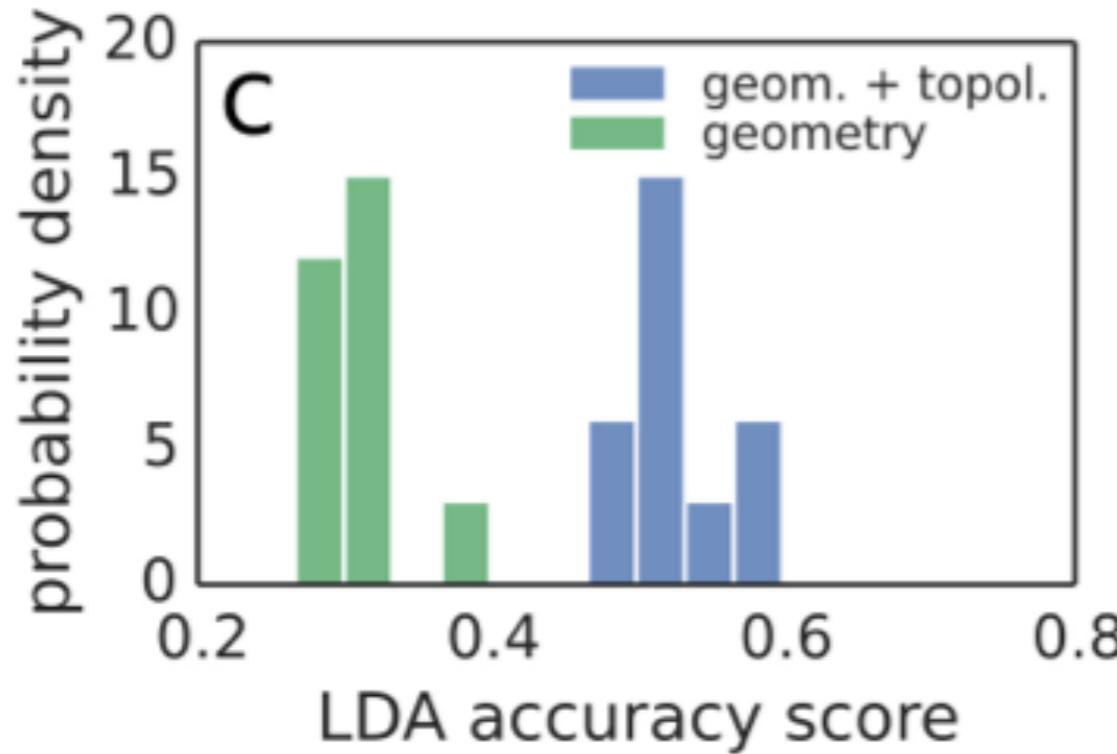
Linear Discriminant Analysis
to identify fragments

supervised learning (attempts to find a set of hyperplanes optimally separating sets of points in a high dimensional space whose class membership is known)



- Two tests:
- (1) identify fragment based on leaf membership (all 186)
 - (2) pairwise comparison test

Leaf fingerprinting

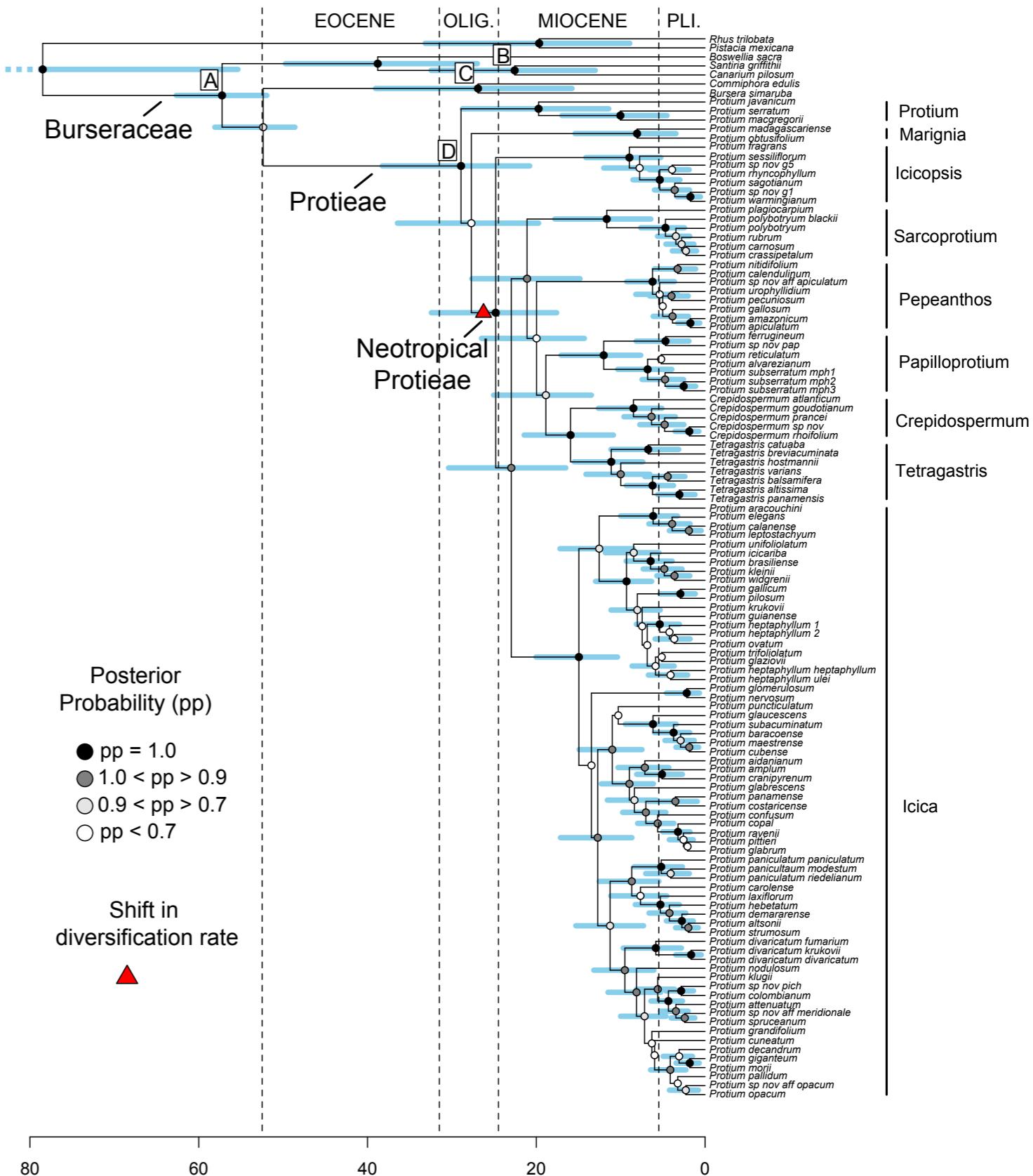


Topological information doubles correct leaf identification probability

Leaf fingerprinting

Comparison to phylogenetic trees?

What can we learn about the evolution of land plants?



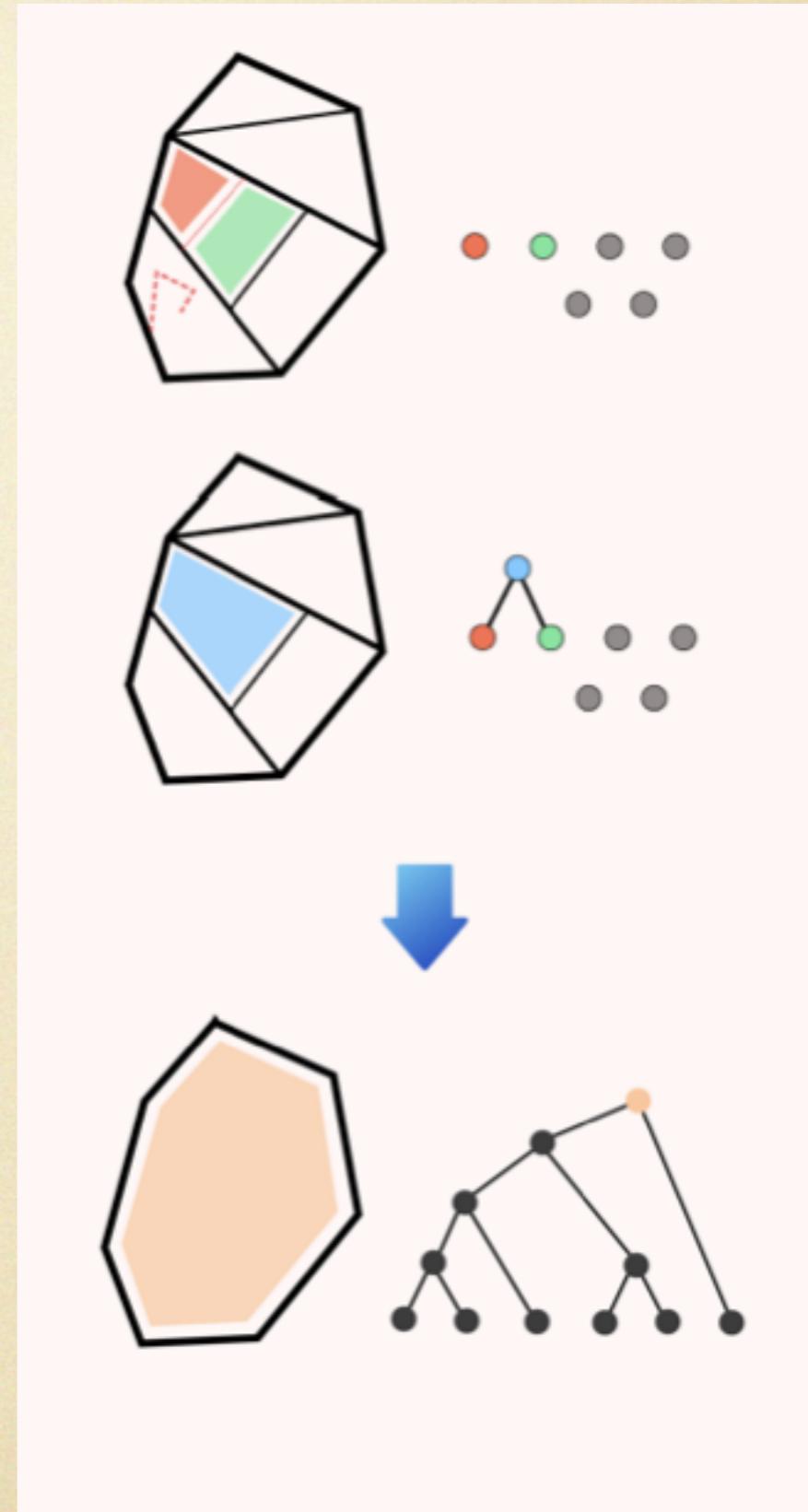
Summary

Sensitive tools are needed to quantify planar graphs of fixed degree.

Topology can offer such tools

“Nestedness” is a distinct phenotype for leaf vascular networks

Method relies on identification of “tiles”. How about 3D?



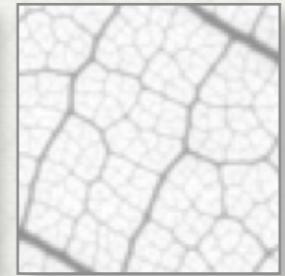
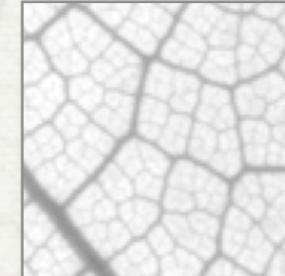
Outline: Quantifying hierarchies in planar graphs

Planar graphs

Motivation

Hierarchical decomposition

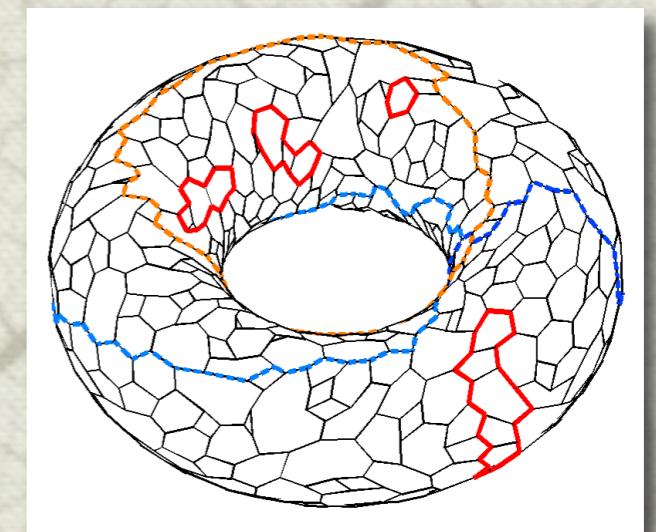
Applications: leaf fingerprinting



Beyond planarity

Every graph can be a planar graph

Applications: transportation systems

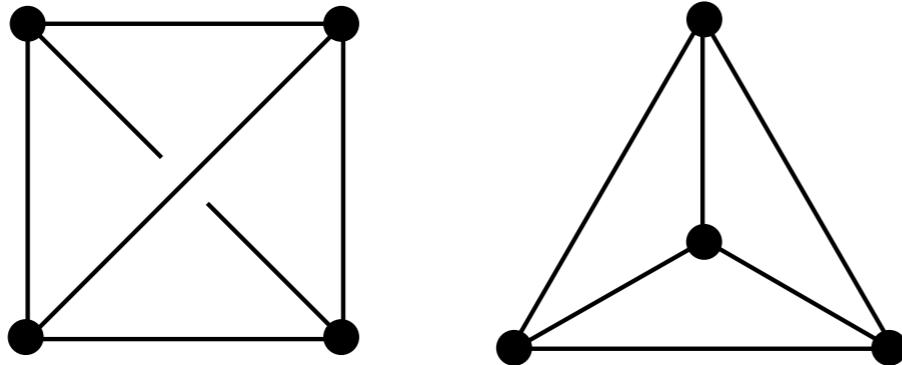


Graph embeddings

Treat 3D graphs as planar

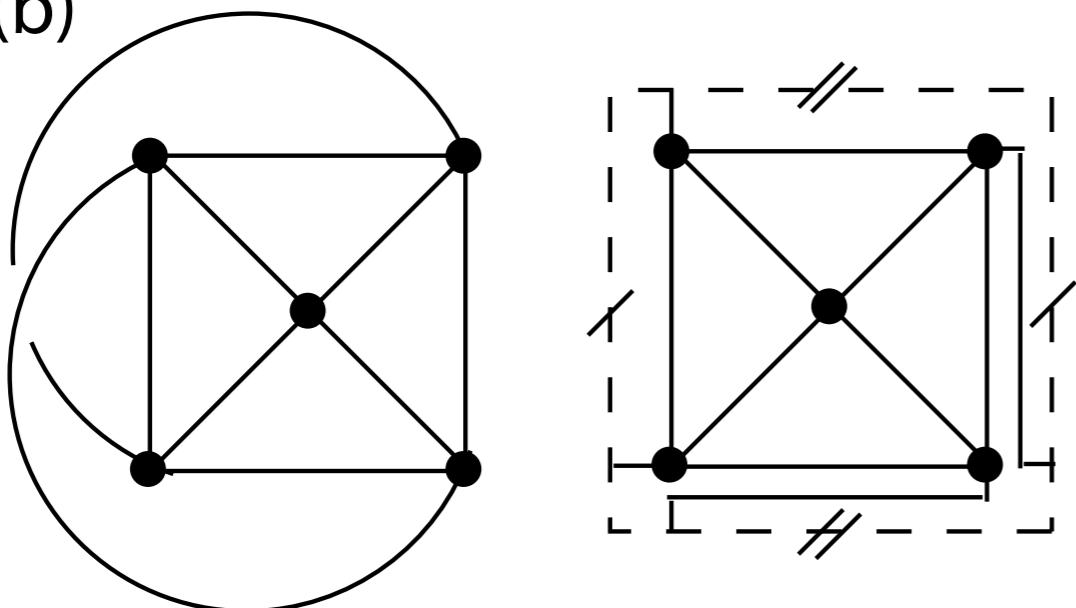
The specific embedding will determine the tiles

(a)



Not embedded in (a), but planar

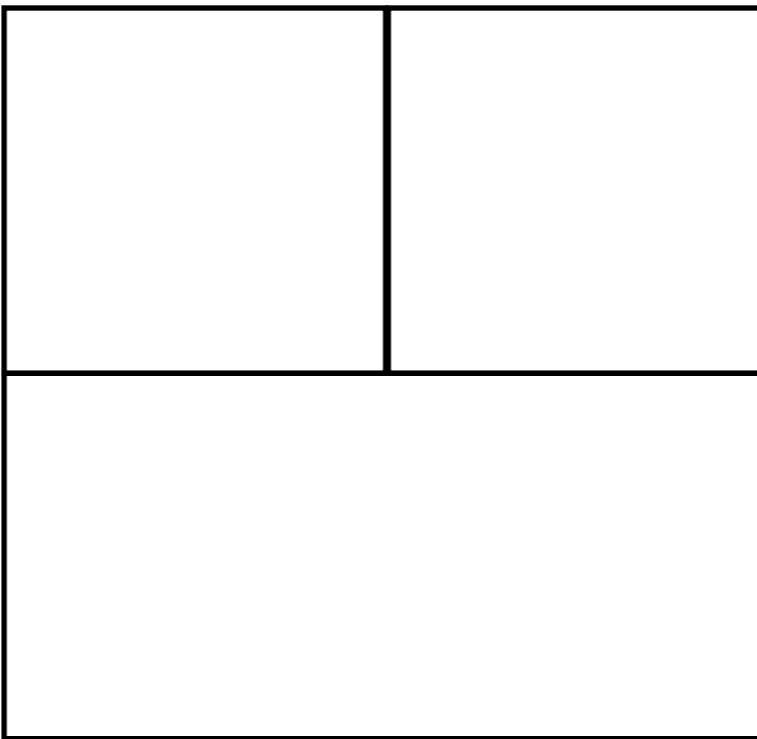
(b)



Not planar, but can be
represented without edge
crossings on a torus.

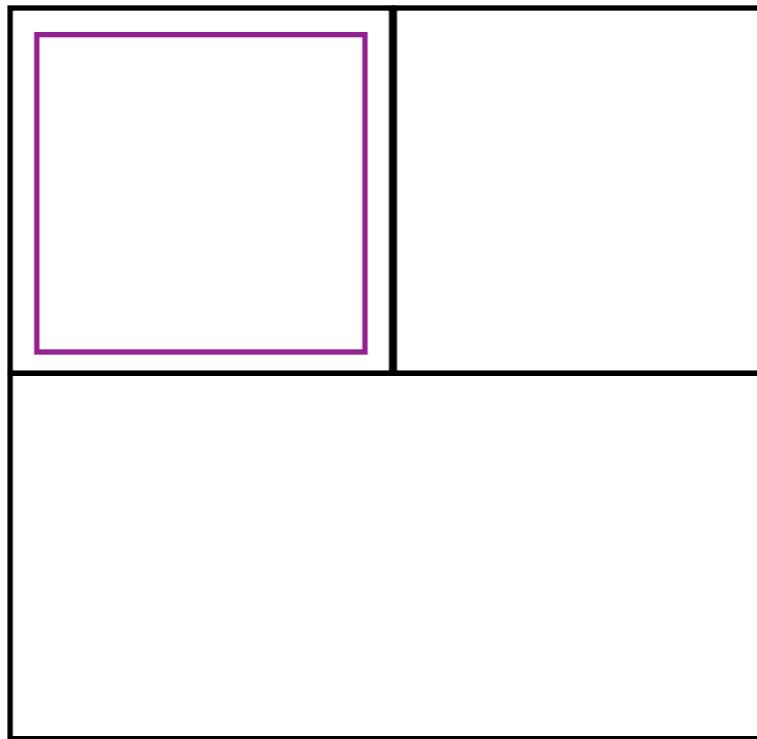
Cycle basis

I can represent all my cycles by addition of the basis cycles



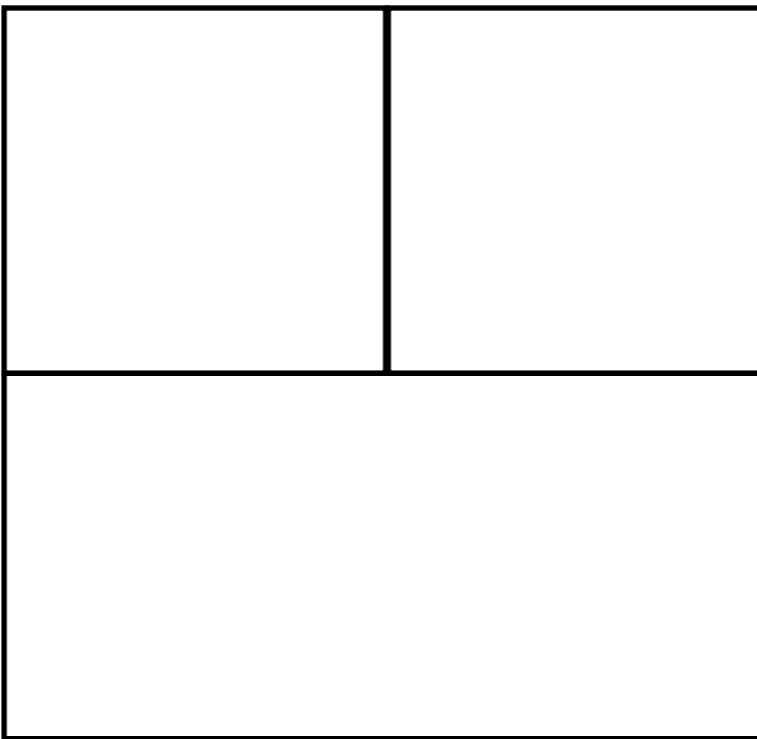
Cycle basis

I can represent all my cycles by addition of the basis cycles



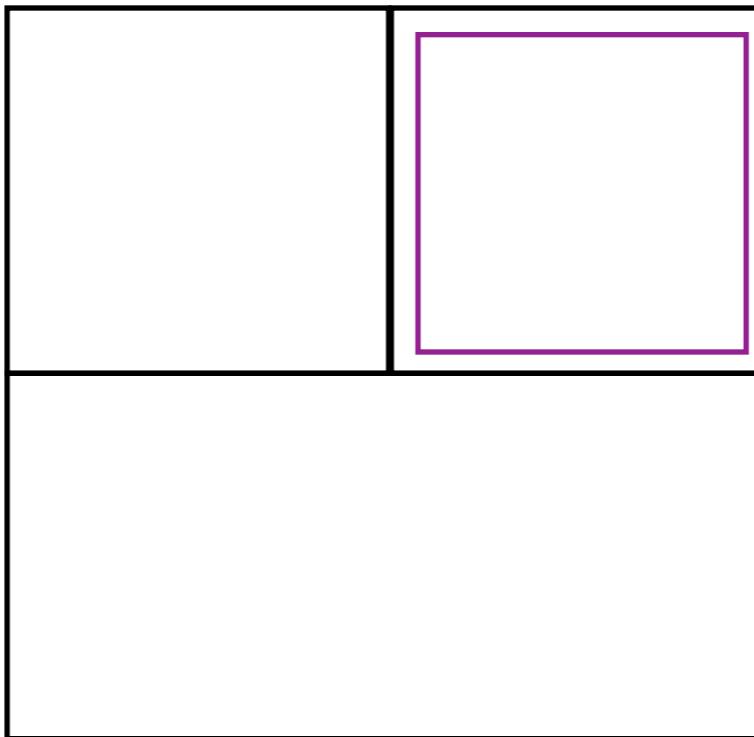
Cycle basis

I can represent all my cycles by addition of the basis cycles



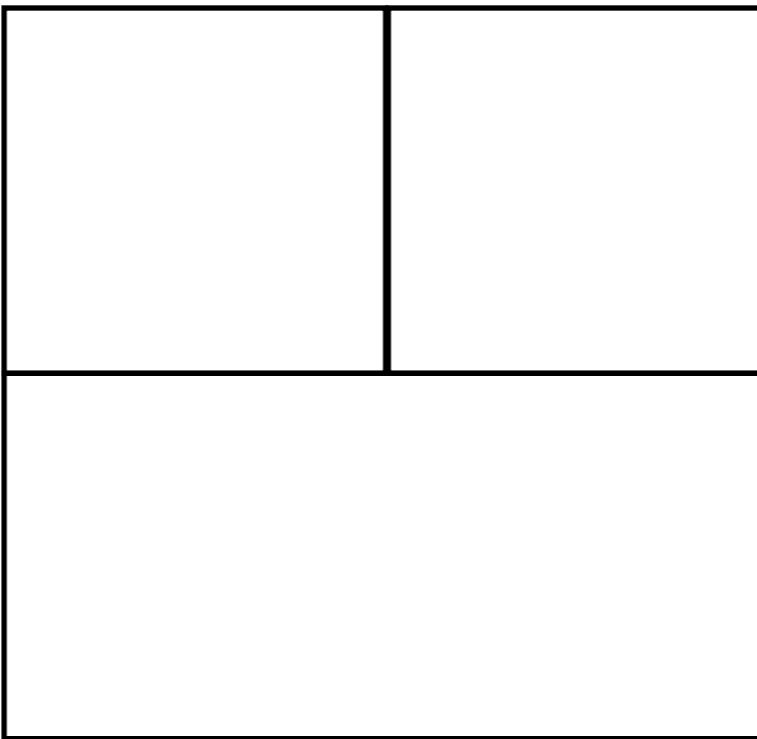
Cycle basis

I can represent all my cycles by addition of the basis cycles



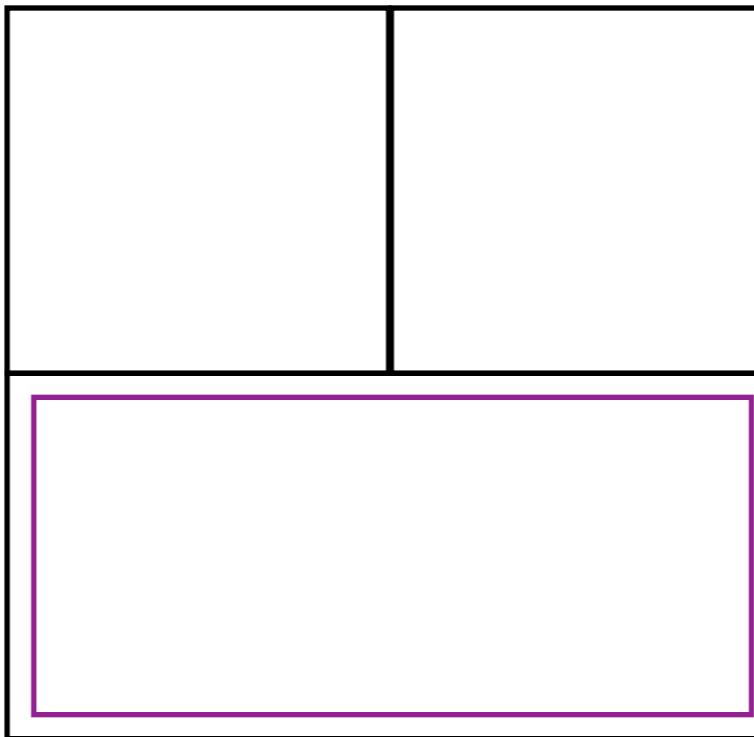
Cycle basis

I can represent all my cycles by addition of the basis cycles



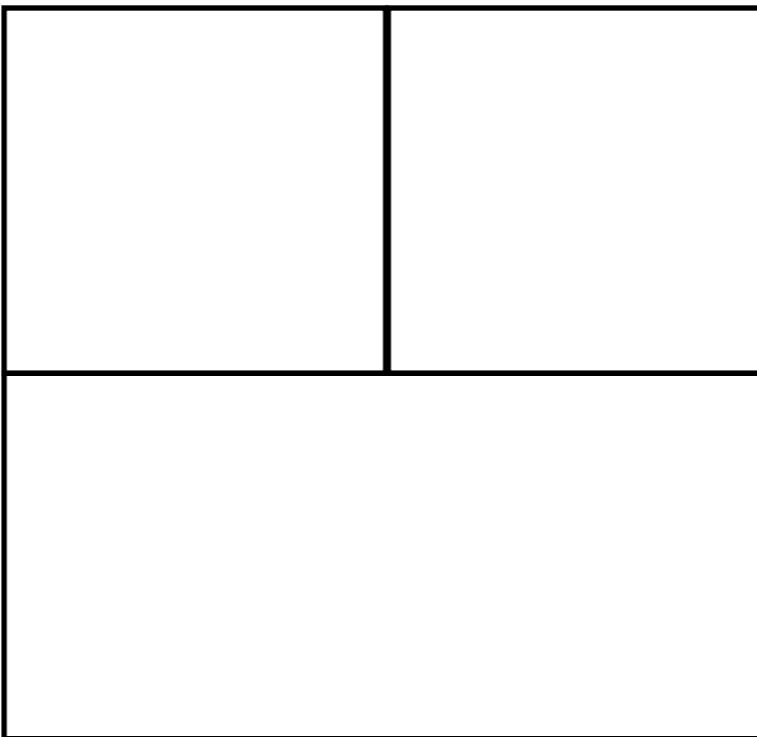
Cycle basis

I can represent all my cycles by addition of the basis cycles



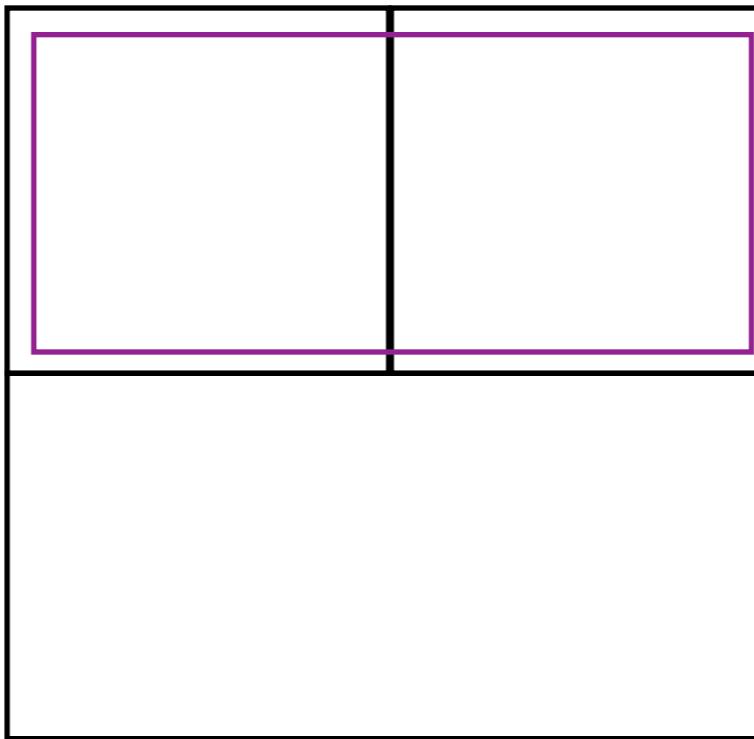
Cycle basis

I can represent all my cycles by addition of the basis cycles



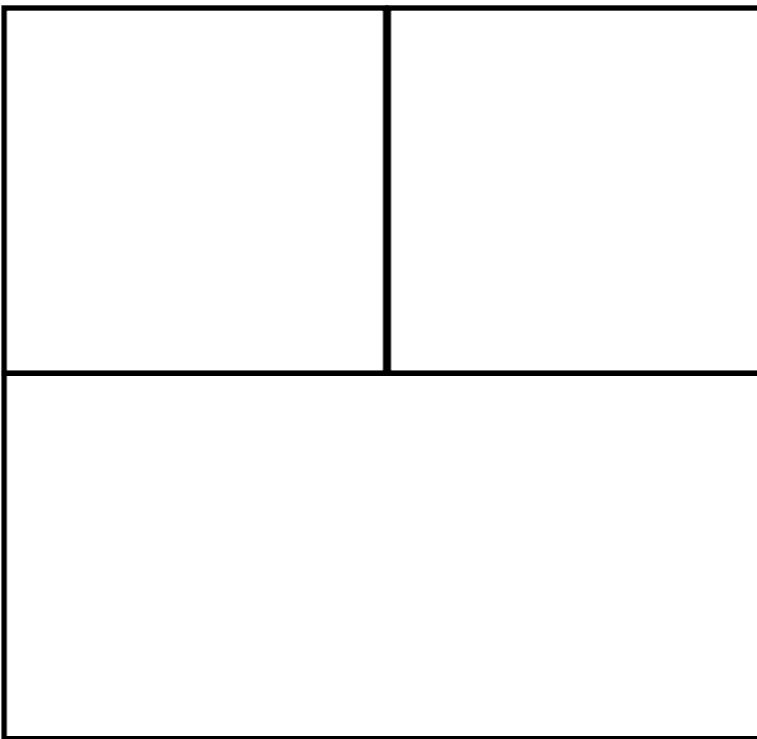
Cycle basis

I can represent all my cycles by addition of the basis cycles



Cycle basis

I can represent all my cycles by addition of the basis cycles

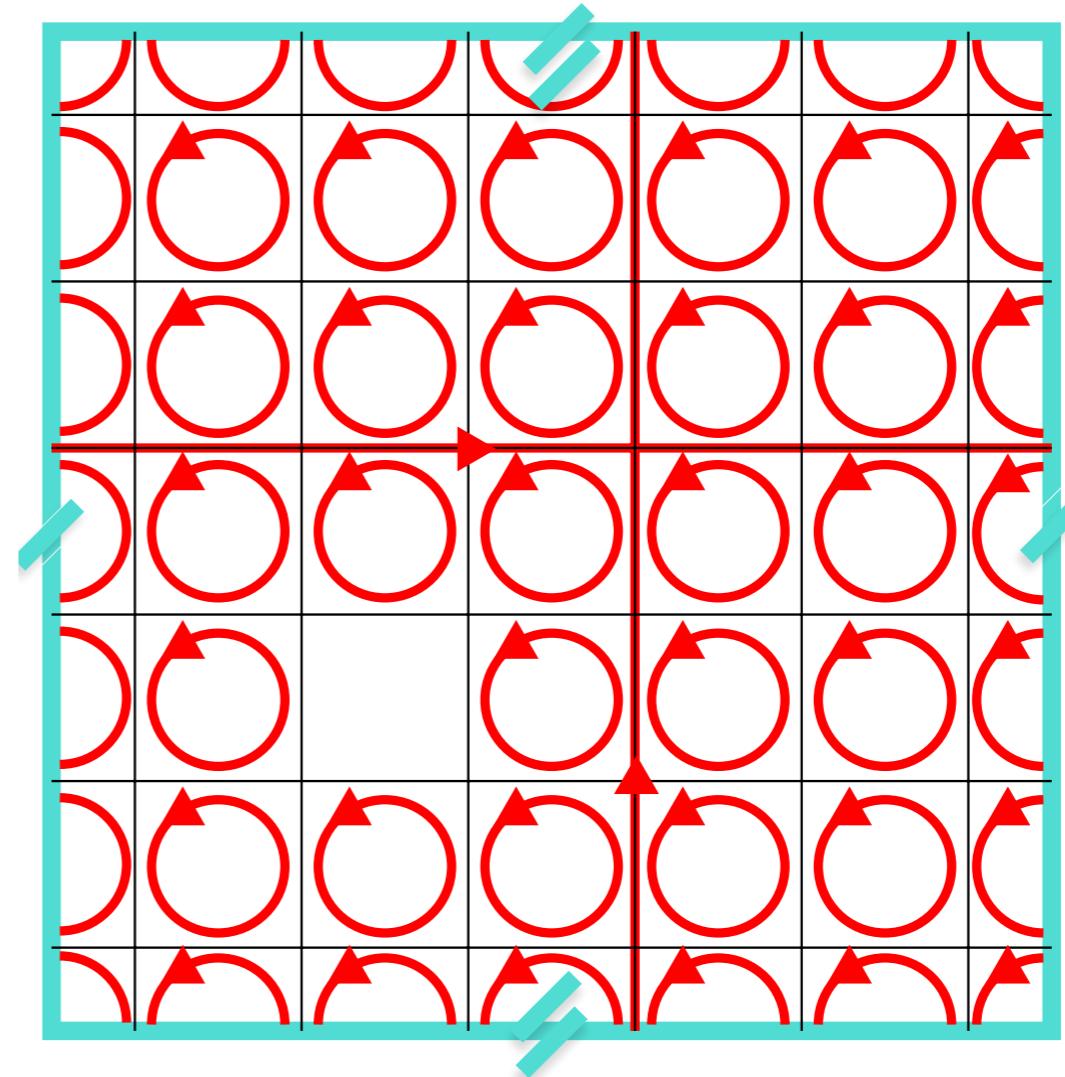
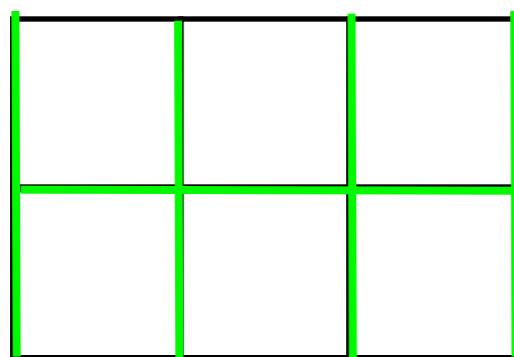


The cycle space

Cycle space: The set of all looped paths without repeated traversal

Vectors: The entire graph with each edge assigned 0 if not traversed and 1 if it is

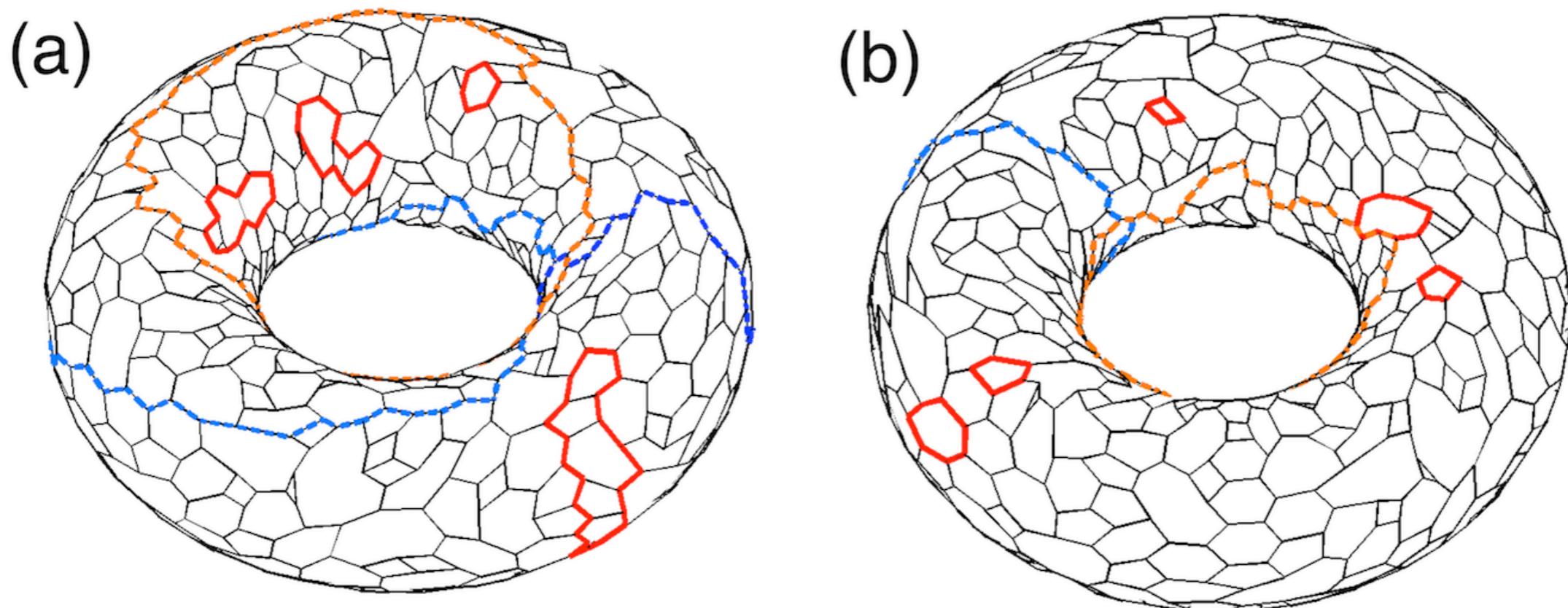
Addition: Simple edge-wise addition (boolean)



$f - 1 = 35$ basis vectors from tiles
 $2g = 2$ basis vectors from generators of π_1

A basis can be constructed by a spanning tree

Finding the minimal basis



Minimum weight basis: J. D. Horton, SIAM J. Comput. 16, 358 (1987)

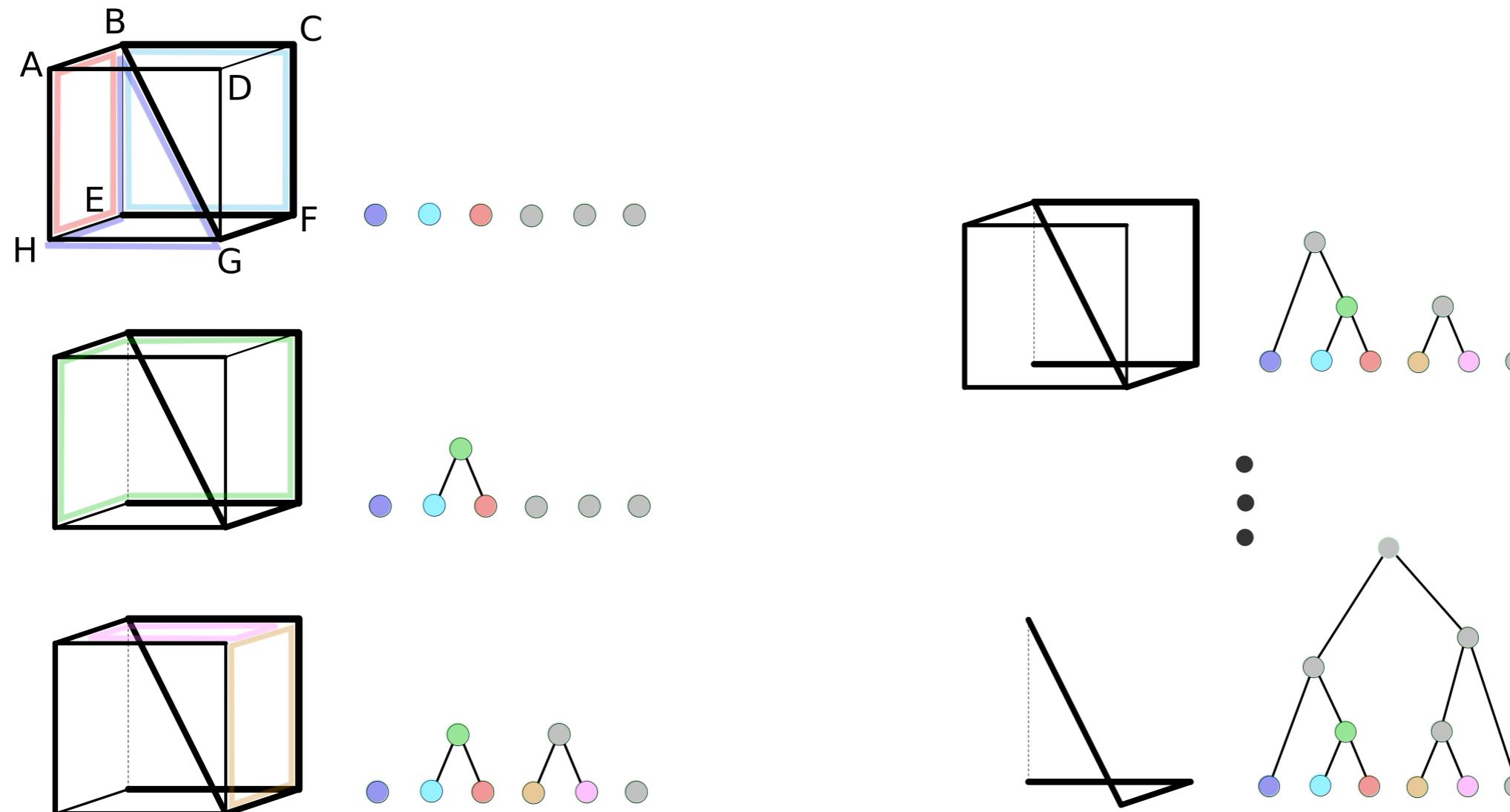
Minimum weight basis: tiling in 2D

Method should only be meaningful if the fundamental (topological) cycles
are much longer than the typical tile size



Constructing the characteristic tree

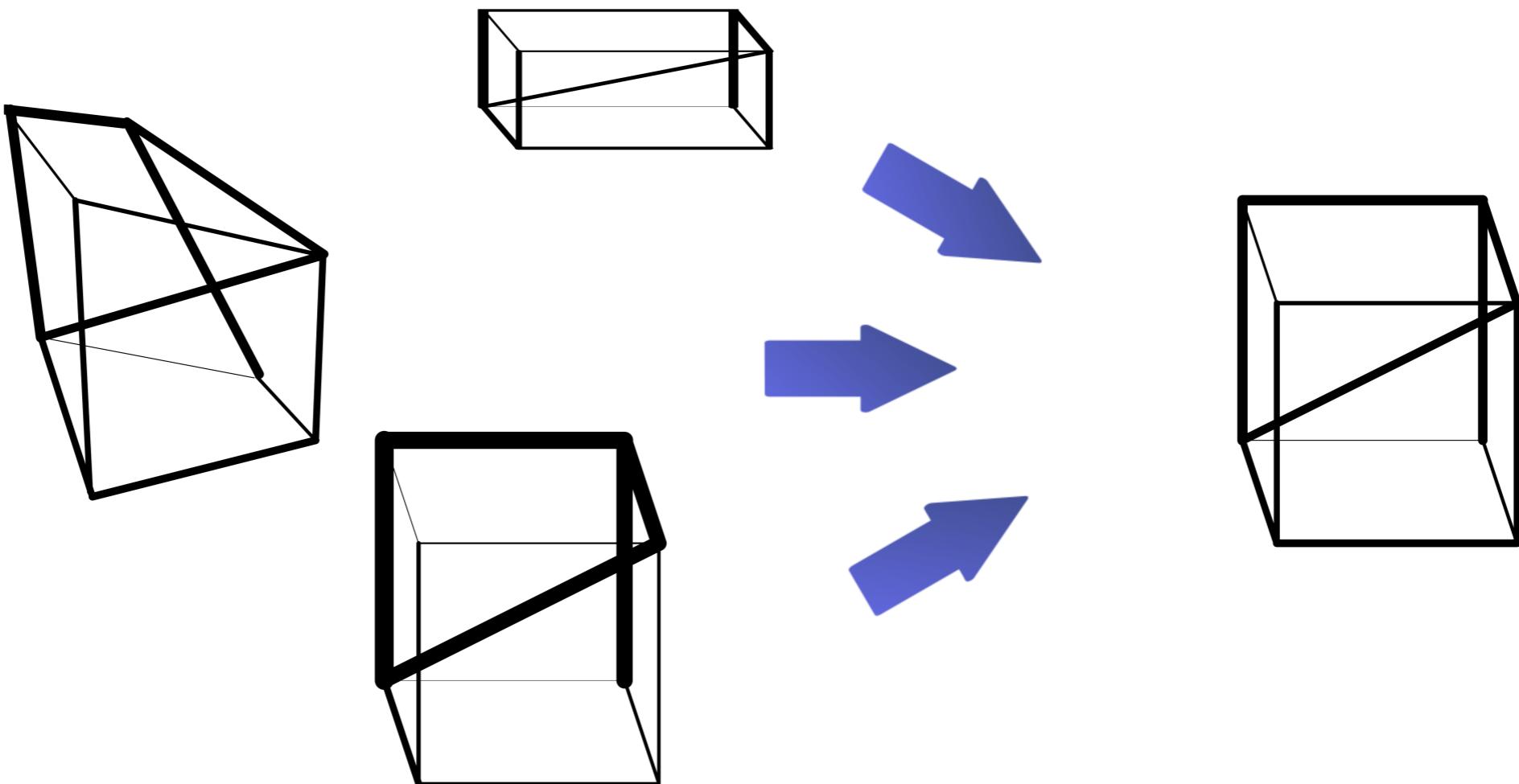
Start with the minimal cycle basis ("tiles") and proceed with hierarchical decomposition



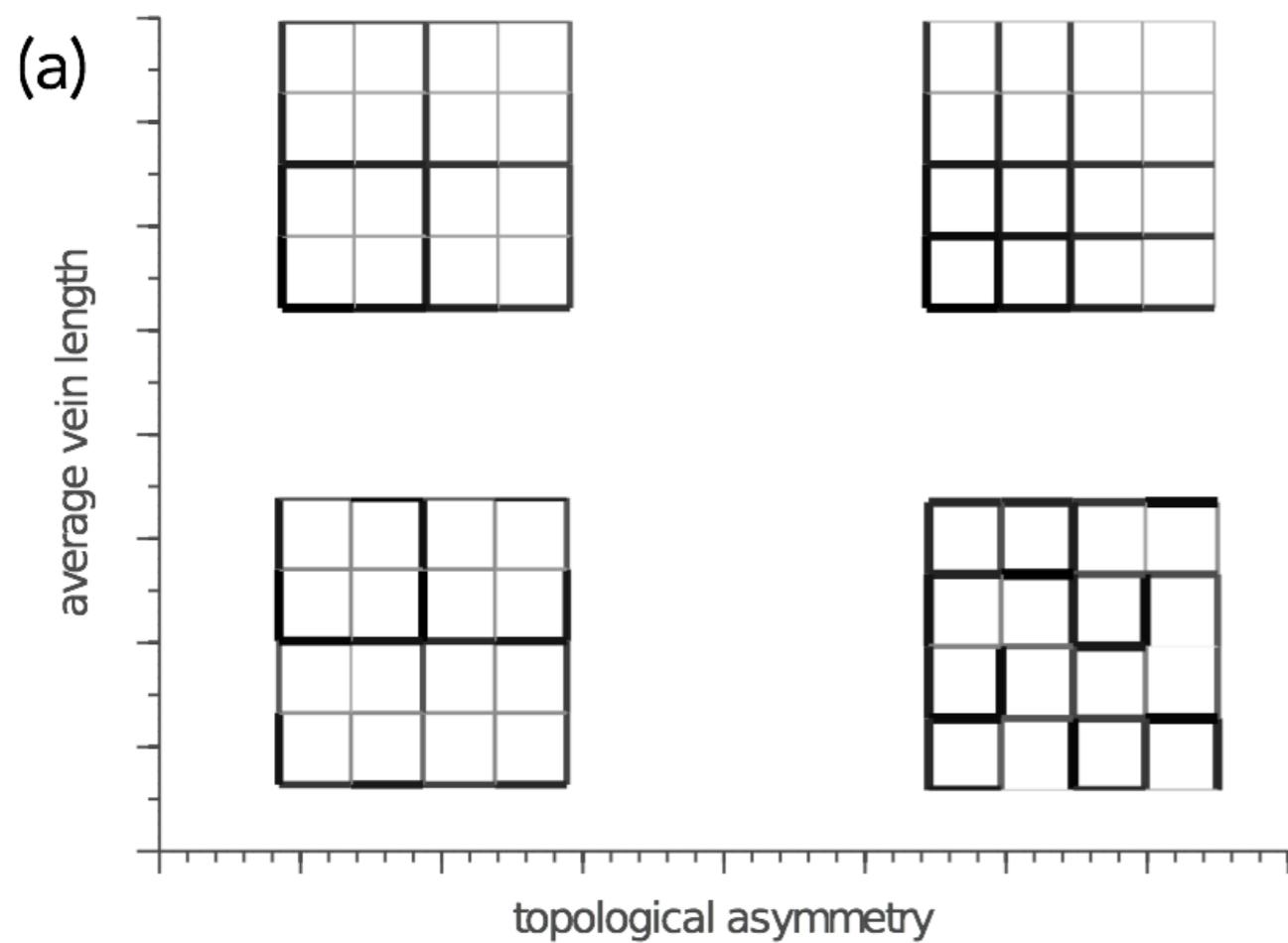
Constructing the characteristic tree

As in planar graphs:

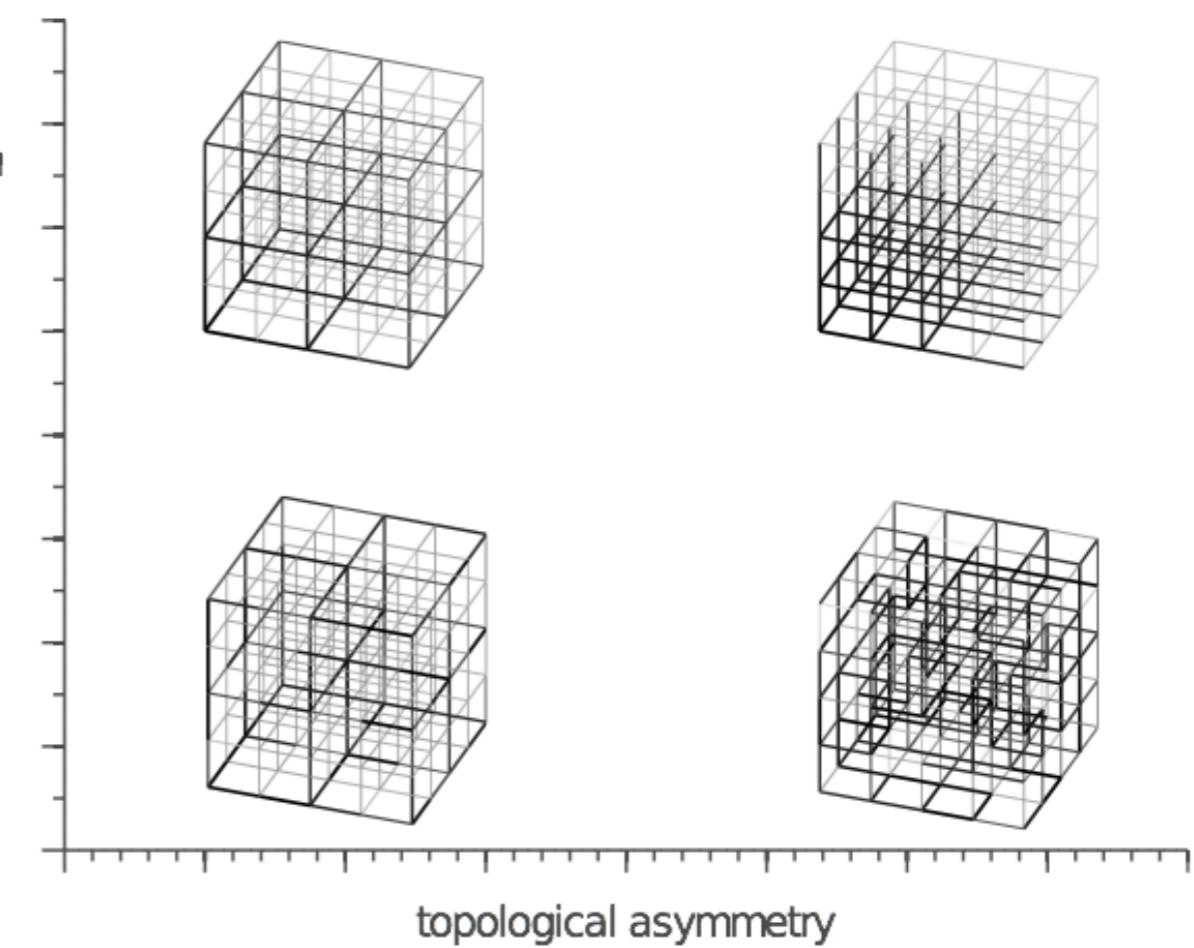
Information about geometry and weight is decoupled
only topology and sort order of edges matters



Graph morphospace



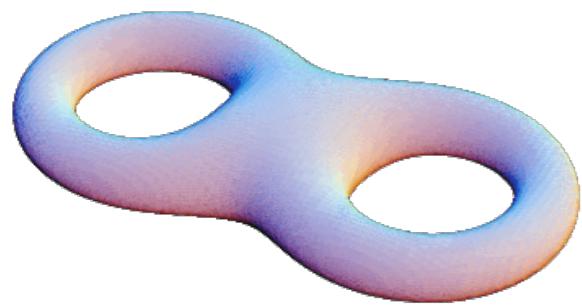
“Phase space” of asymmetry
and average vein length



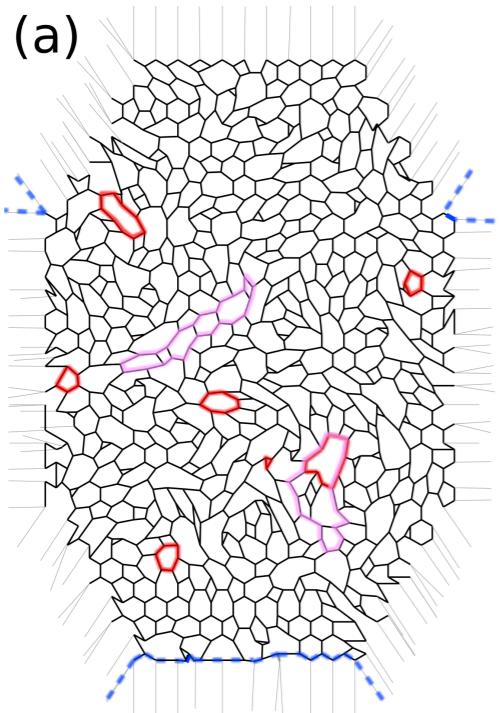
Example networks

Two different underlying topologies

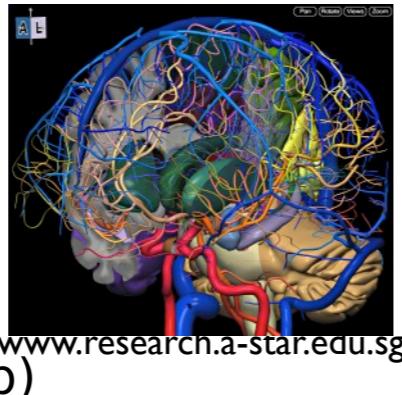
Two handle torus
(known embedding)



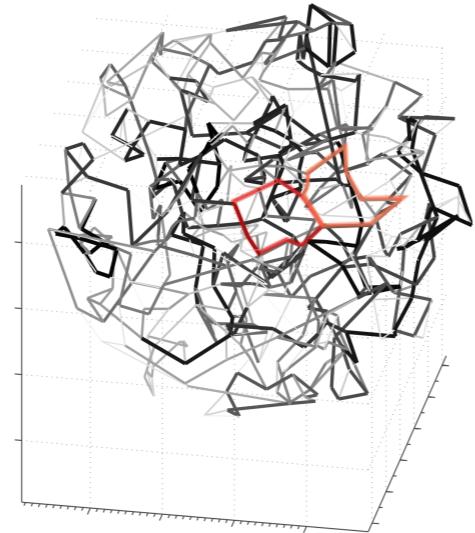
(a)



Random 3D
(physiological)

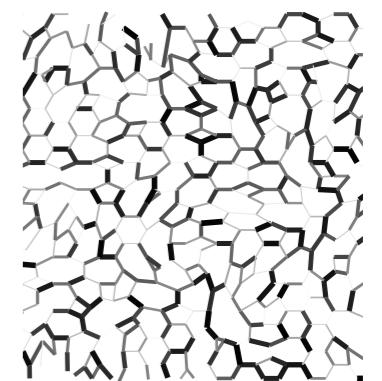


(b)

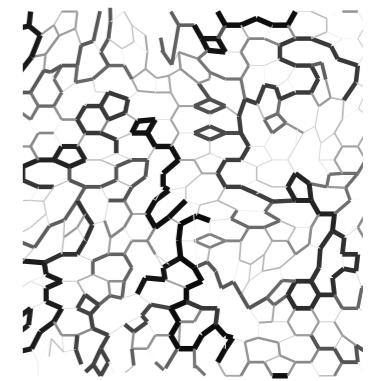


Three different edge weight distribution algorithms

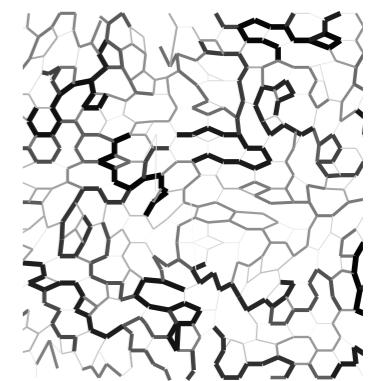
random



lines



lines with SA



Example networks

Adaptive networks

$$Q_{ij}^{kl} = \frac{C_{ij}}{l_{ij}} \cdot (p_i^{kl} - p_j^{kl})$$

$$\langle |Q_{ij}| \rangle := \frac{1}{\frac{N \cdot (N-1)}{2}} \sum_{(k,l) \in \mathbb{P}} |Q_{ij}^{kl}|$$

decay term

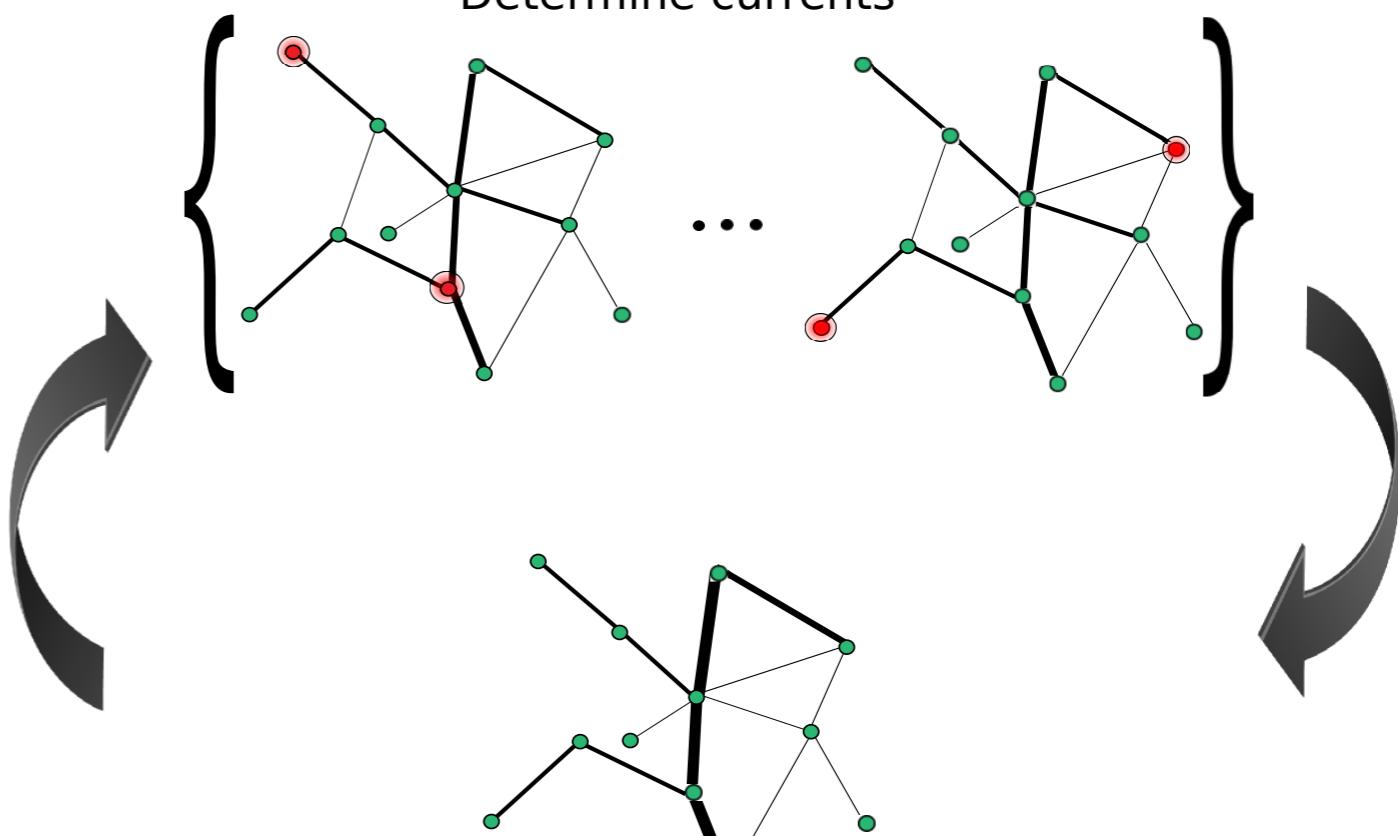
$$\frac{dC_{ij}(t)}{dt} = \beta \cdot f\left(\frac{\langle |Q_{ij}(t)| \rangle}{\epsilon}\right) - \alpha \cdot C_{ij}(t)$$

Local positive feedback

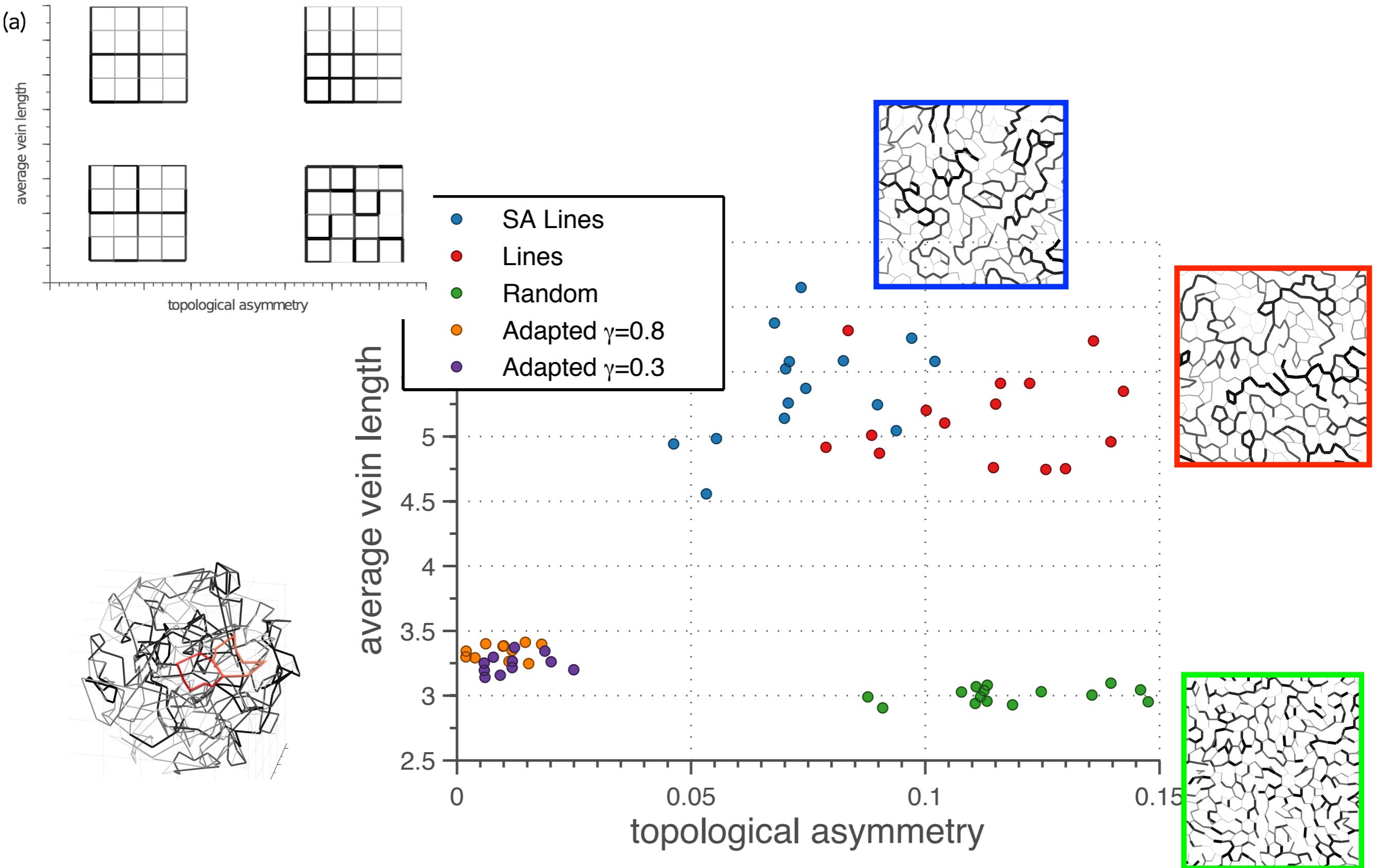
Update model

Determine currents

Update link weights

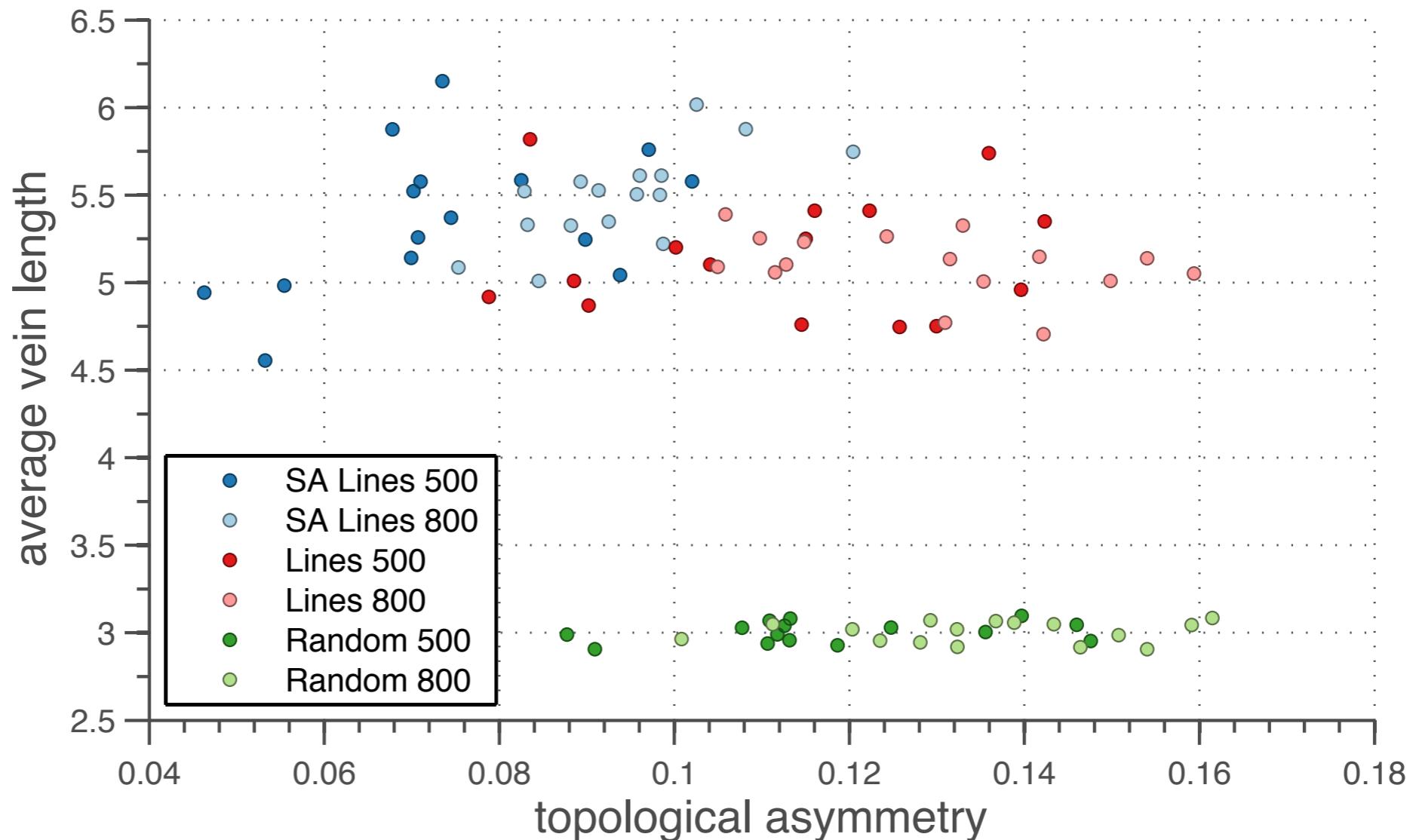


Graph morphospace



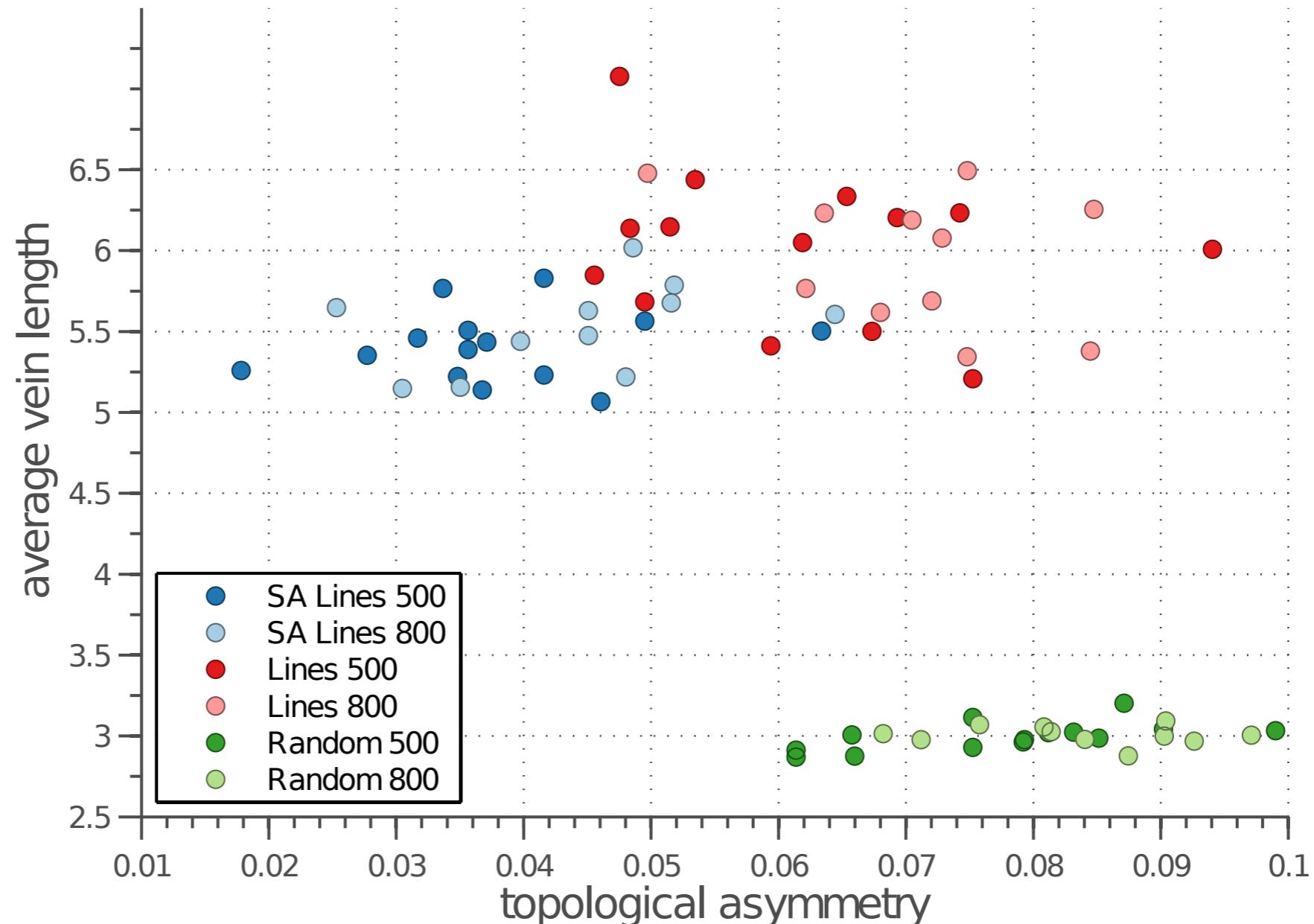
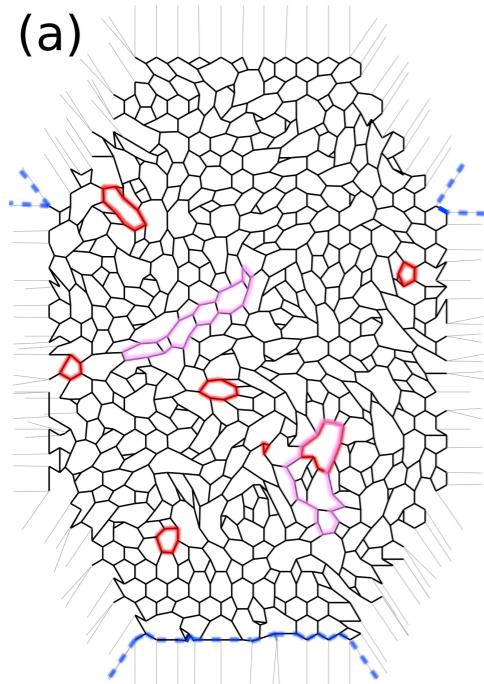
Graph morphospace

Robust to size differences



Graph morphospace

Robust to underlying topology differences

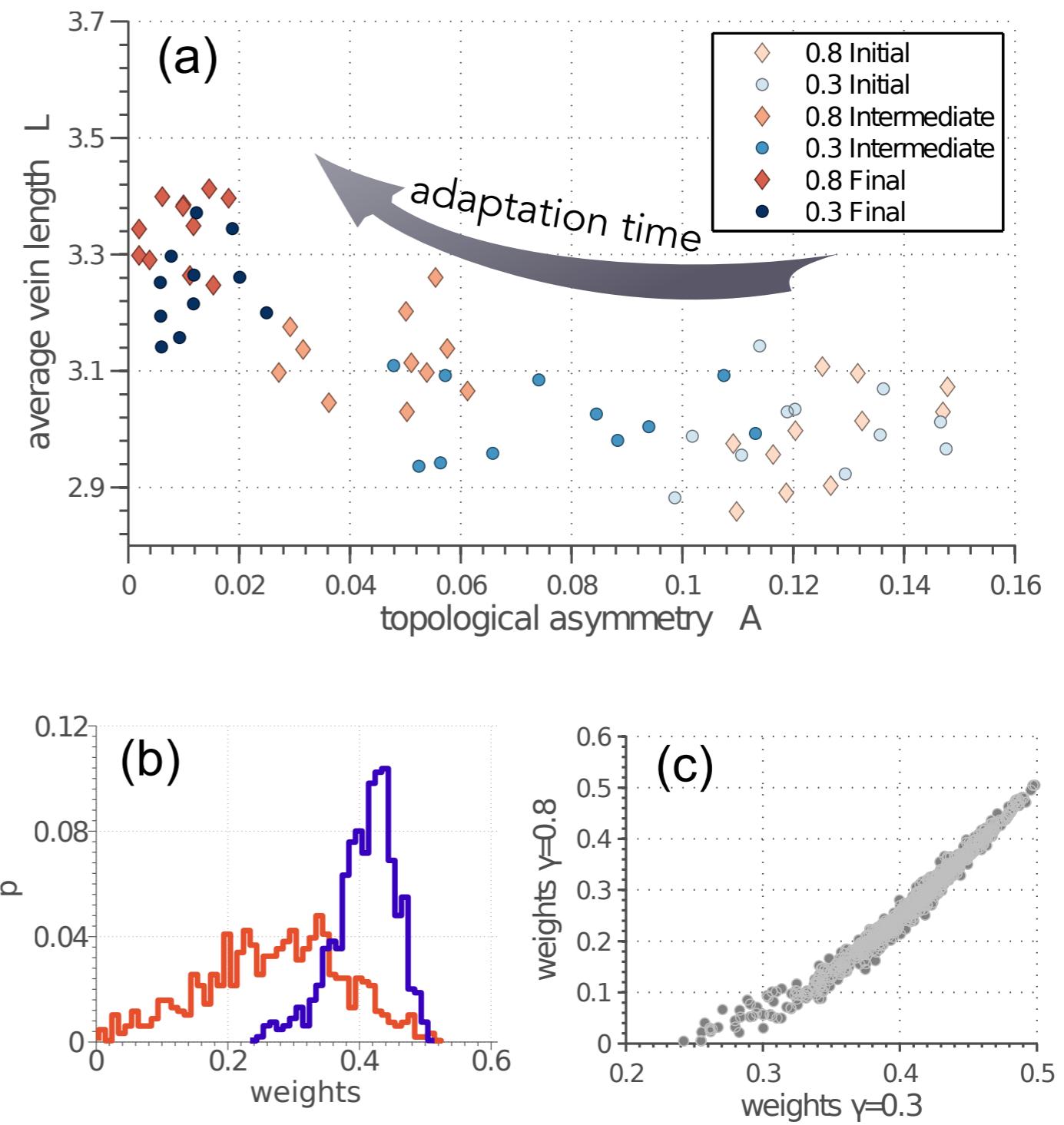


Adaptation dynamics

Different feedback terms produce similar topology, but very different weight distributions

$$\frac{dC_{ij}(t)}{dt} = \beta \cdot f\left(\frac{\langle |Q_{ij}(t)| \rangle}{\epsilon}\right) - \alpha \cdot C_{ij}(t)$$

Feedback term $f(x) = \frac{x^\gamma}{1+x^\gamma}$

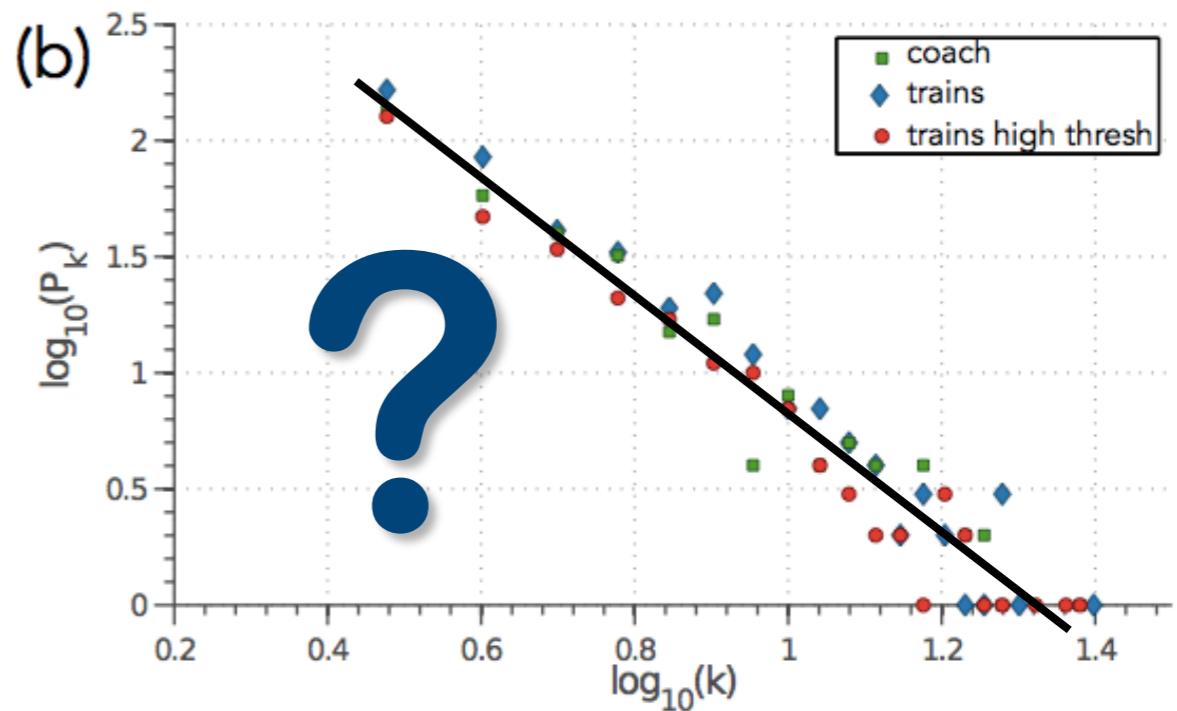
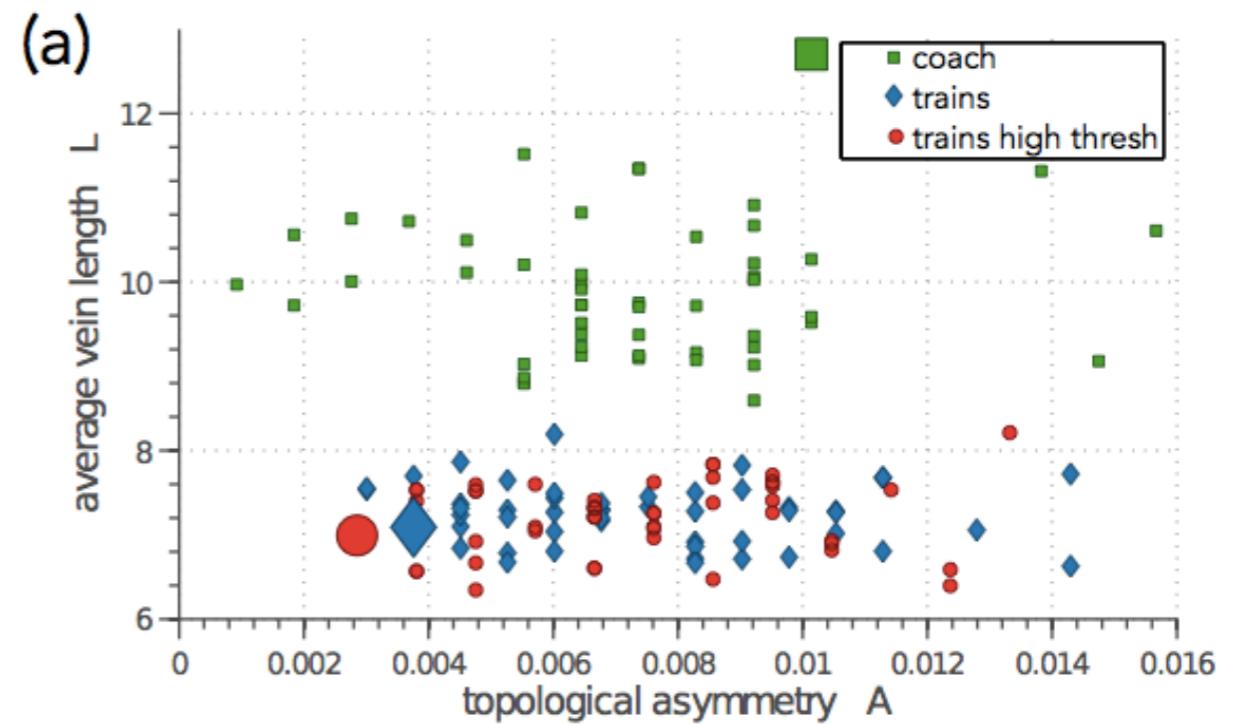
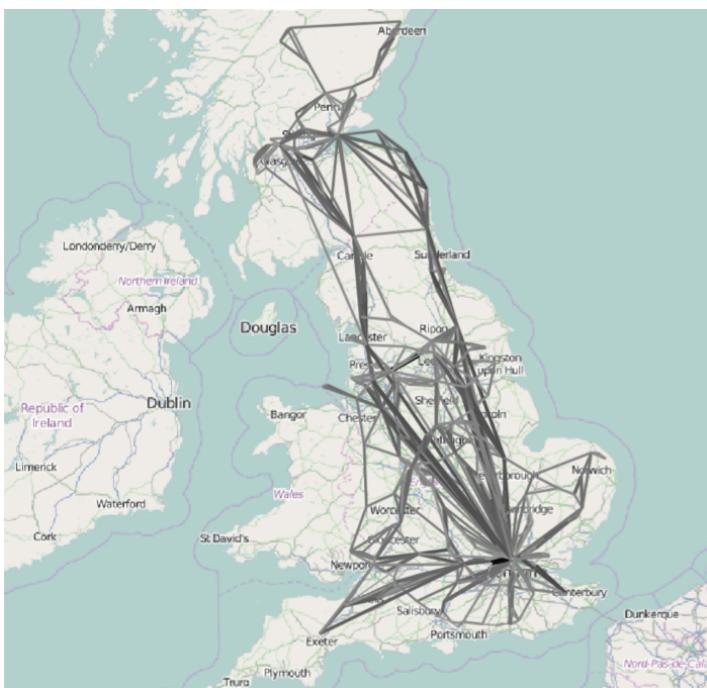


Applications to transport systems

UK coach



UK train

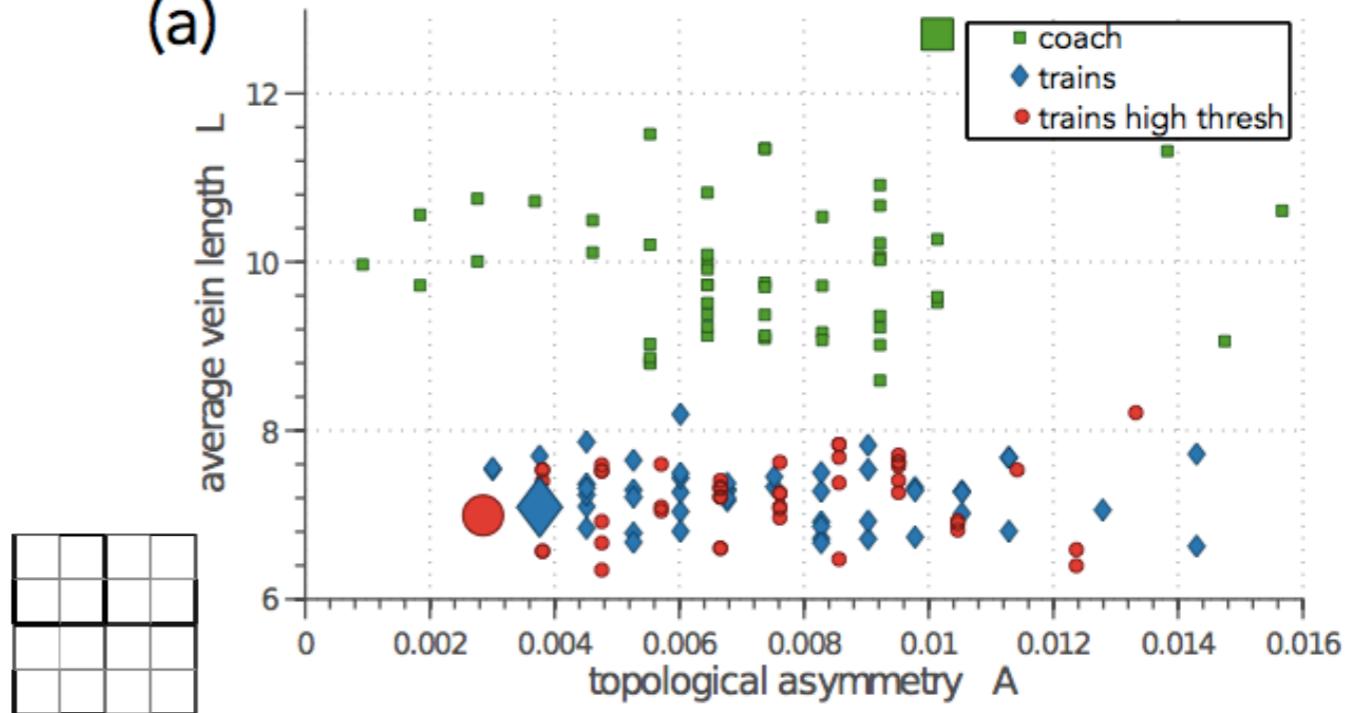


Applications to transport systems

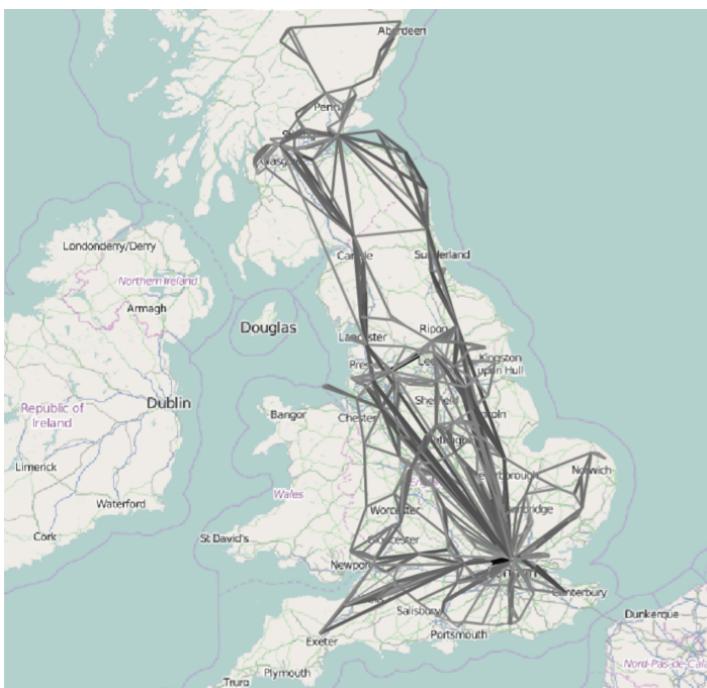
UK coach



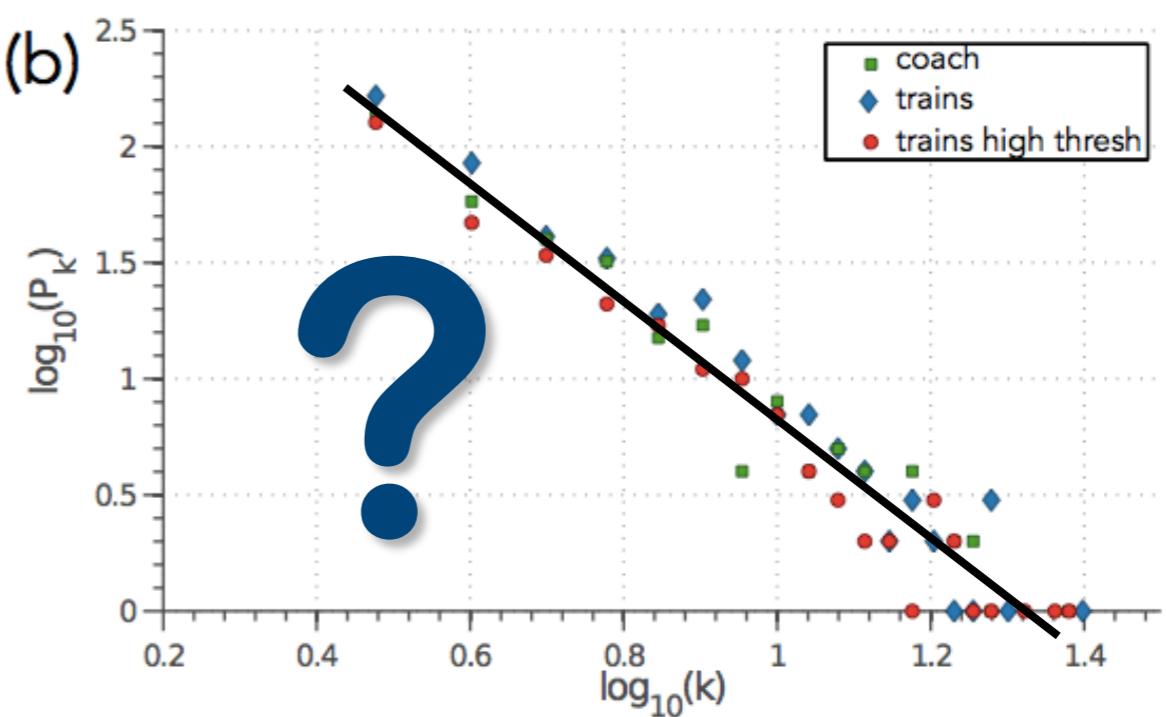
(a)



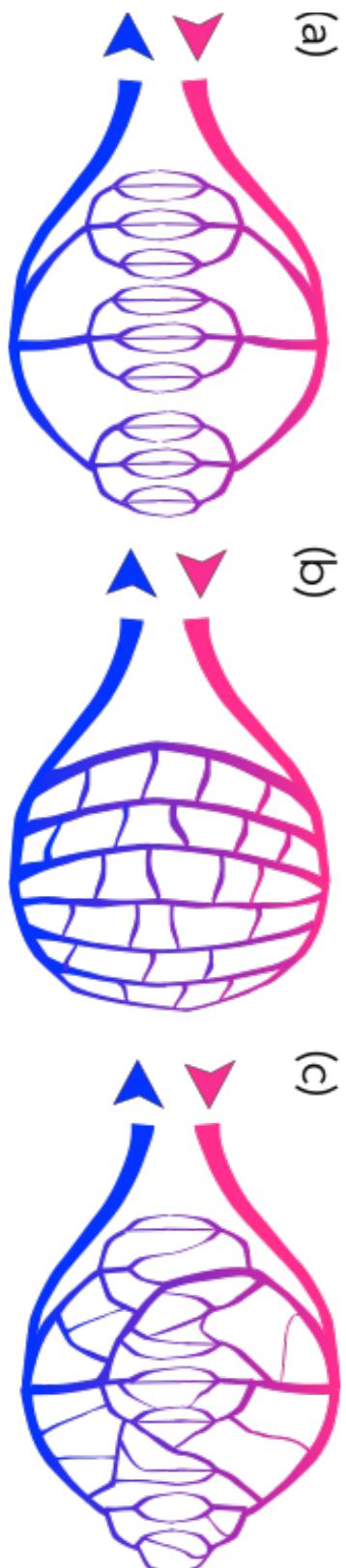
UK train



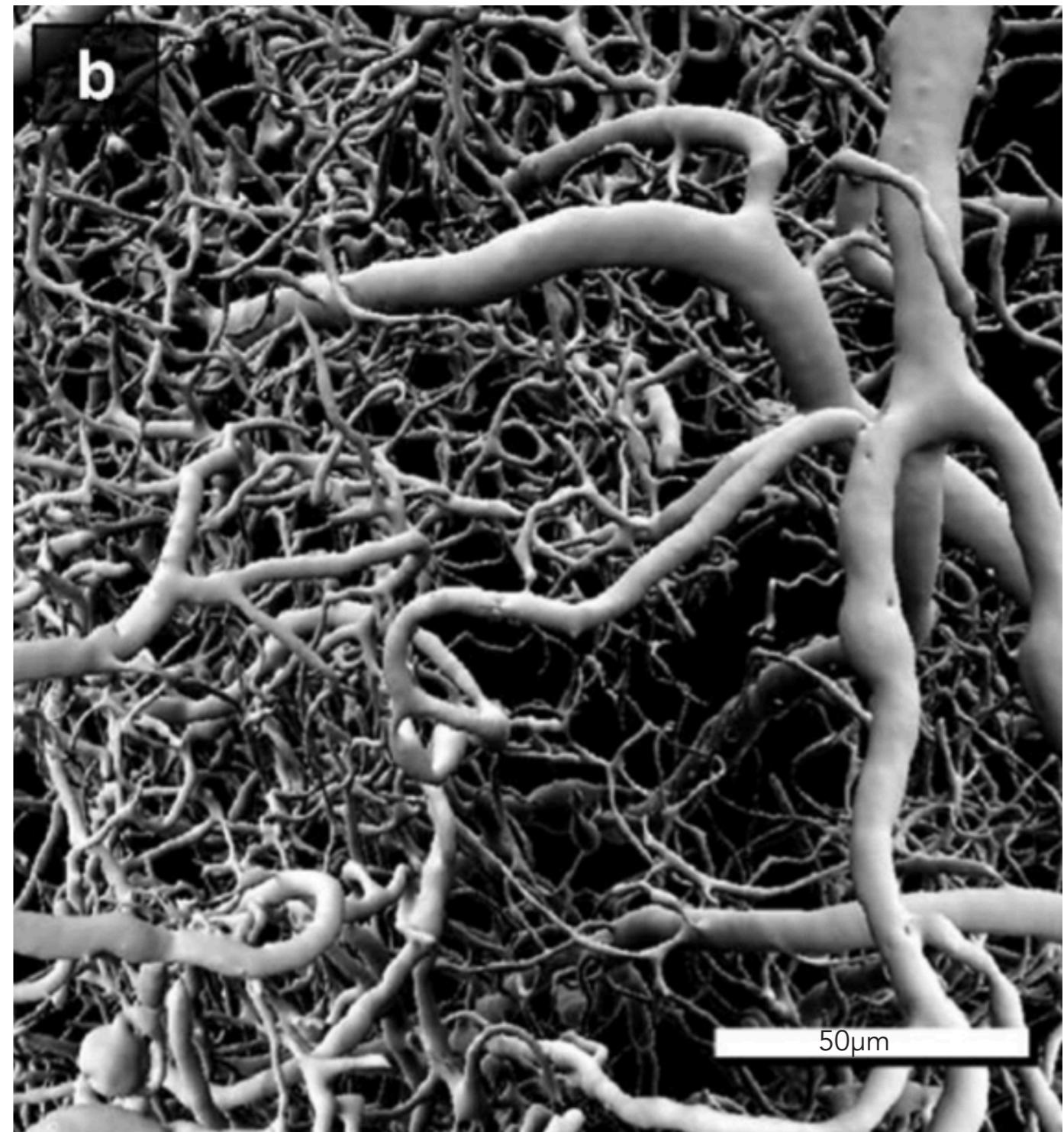
(b)



Applications to vasculature



What are the right metrics to identify disease?

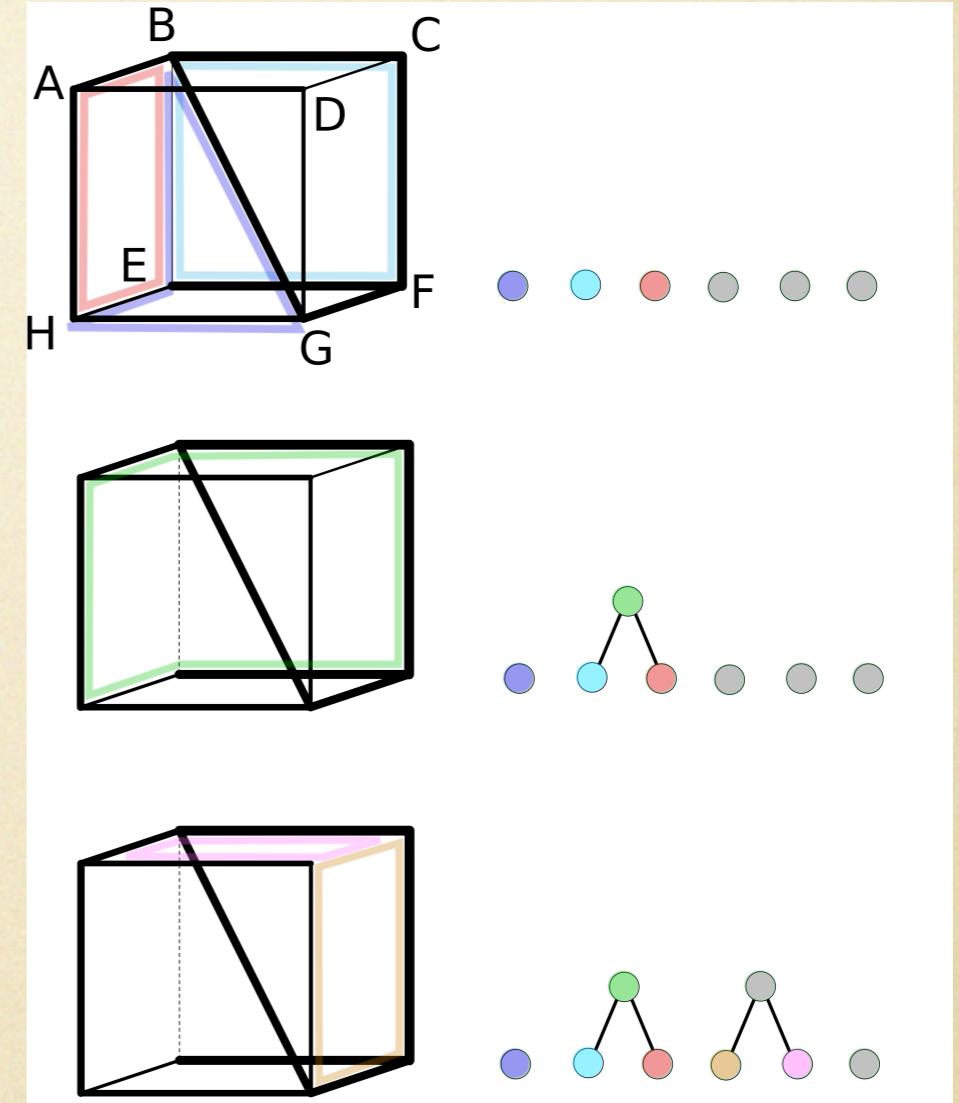


Summary

A non-planar graph of near fixed degree can be considered as tiling the surface of a surface of sufficiently high genus.

The minimal cycle basis is as a good approximation (statistically) for that tiling.

Cycle nestedness offers a new way to look at the hierarchical organization of loopy graphs



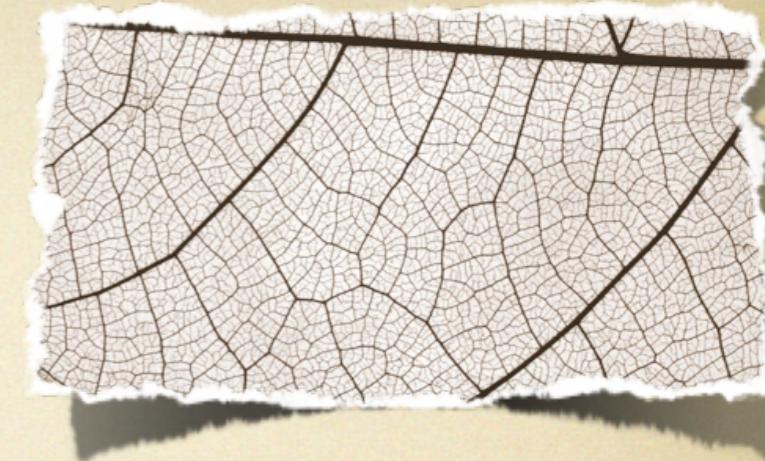
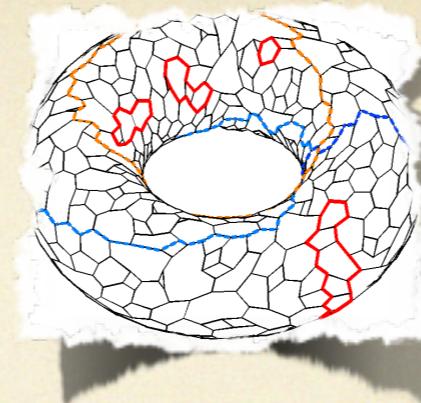
Douglas Daly (New York Botanical Garden)

Marcelo Magnasco (Rockefeller NY)

Carl Modes (Rockefeller NY)

Jana Lasser (MPI DS)

Henrik Ronellenfitsch (MPIDS)



Theory

EK. and Magnasco M.O., "Quantifying loopy network architectures", *PLoS ONE*, 7, e37994 (2012)

Modes C. D., Magnasco M.O., and EK., "Extracting Hidden Hierarchies in 3D Distribution Networks", *under review* <http://lanl.arxiv.org/abs/1410.3951>

Applications

Ronellenfitsch H. Lasser J., Daly D., and EK, "Topological phenotypes of leaf vascular networks", *submitted*

Network extraction and image processing

Lasser J., EK, "NEAT: A new framework for the vectorization and examination of network data", *in preparation,*

[https://github.com/JanaLasser/network_extraction.](https://github.com/JanaLasser/network_extraction)



Thank you!

Bonus material



Statistics of the tiling

Statistically 'real' tiles should be shorter than cycles that traverse entire 'handles' of the surface.

$$2 - 2g = V - E + F$$

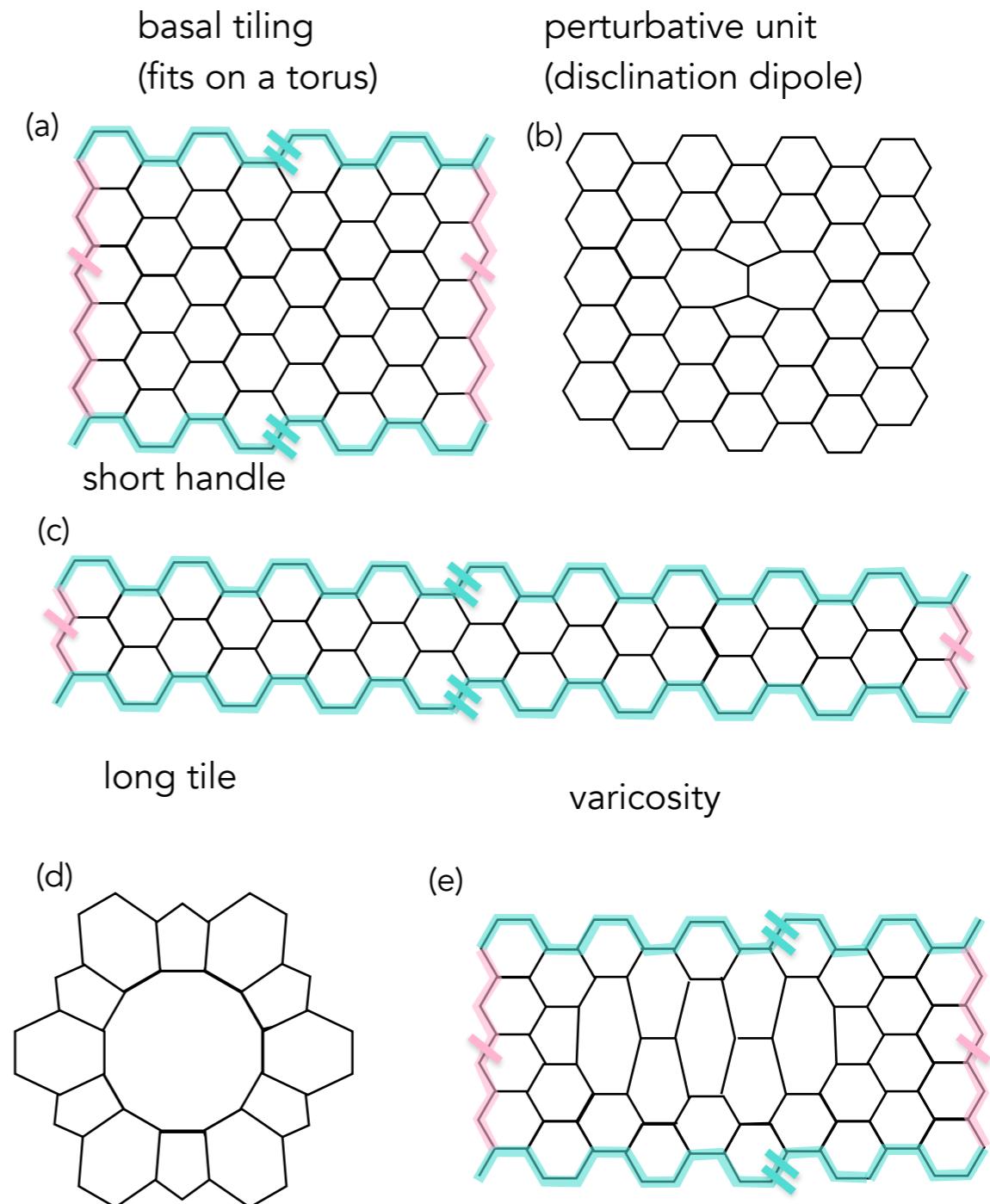
3-regular graphs $E = 3V/2$.

Average number of edges / tile $|p|$

$$|p|F = 2E$$

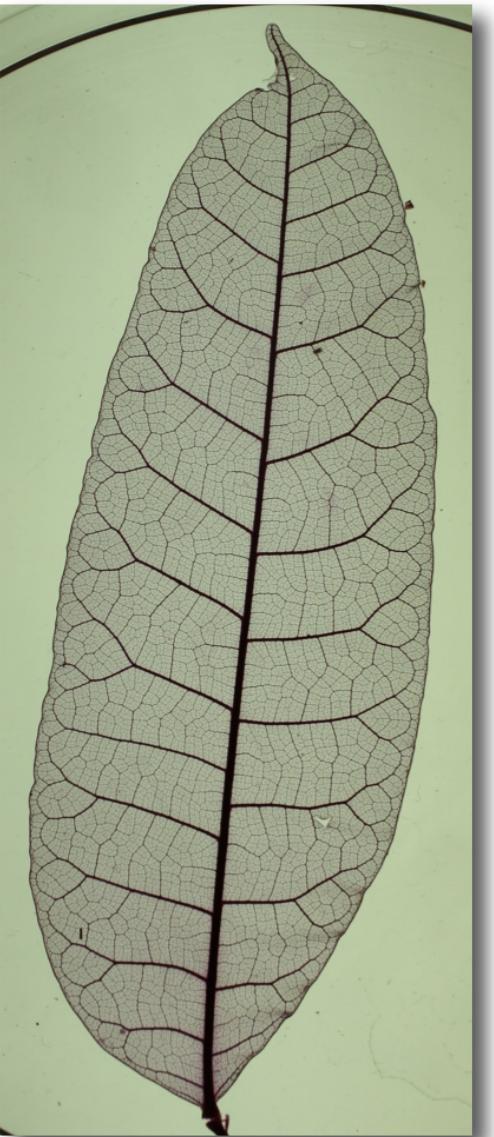
$$|p| = \frac{6V}{4 + V - 4g}$$

For fixed V , a surface may be represented as a $4g$ -gon with appropriate sides identified $V^{1/2}/g$.

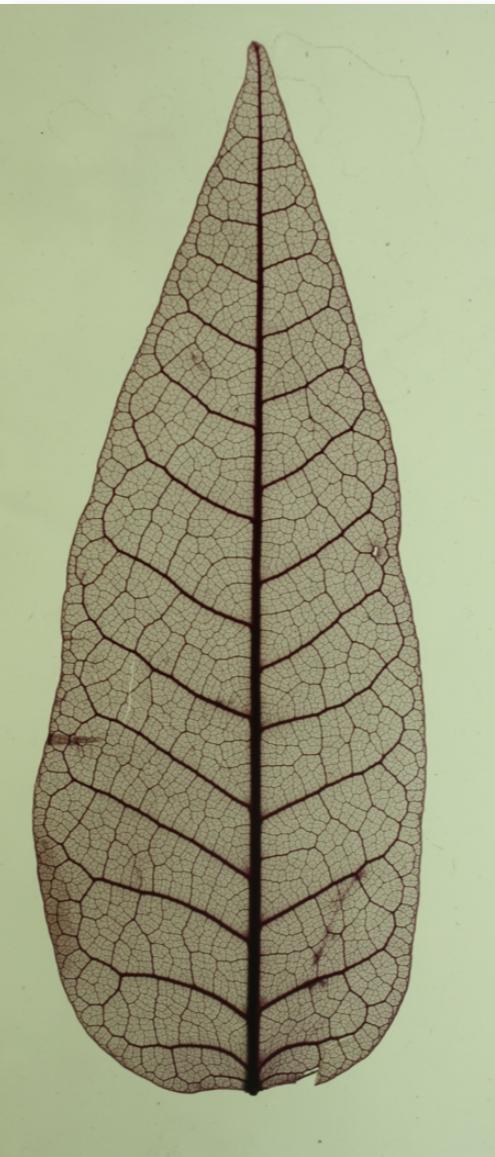


Deciphering the topology

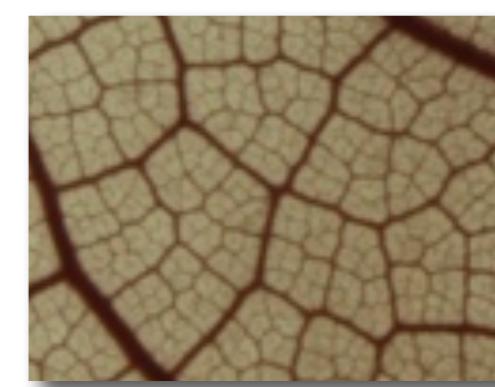
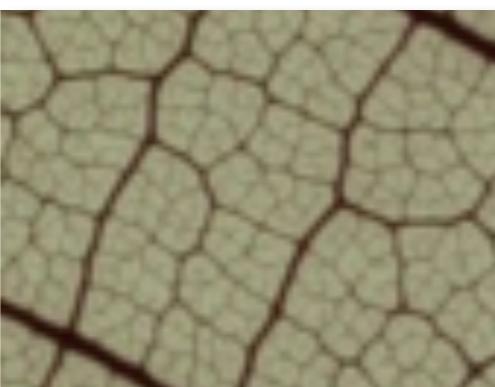
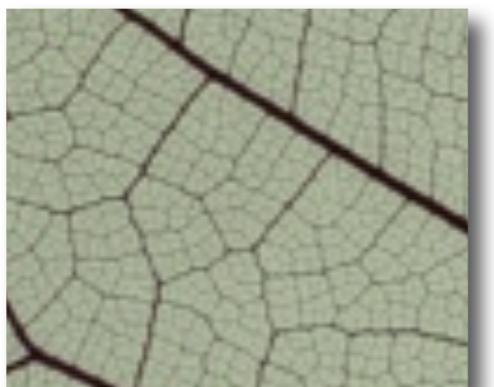
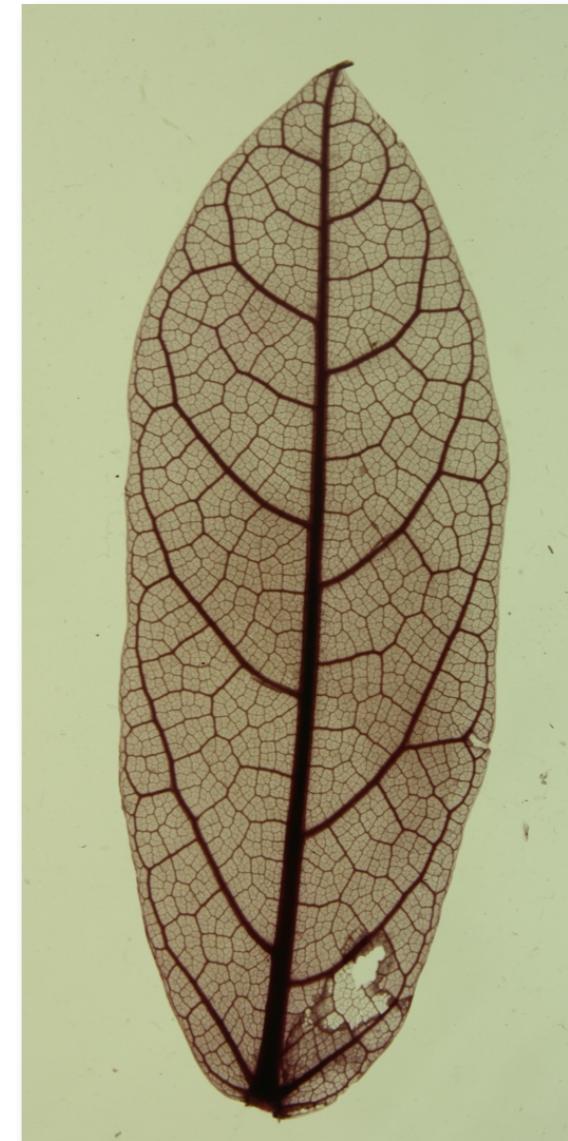
Canarium altissima



Canarium multiflorum

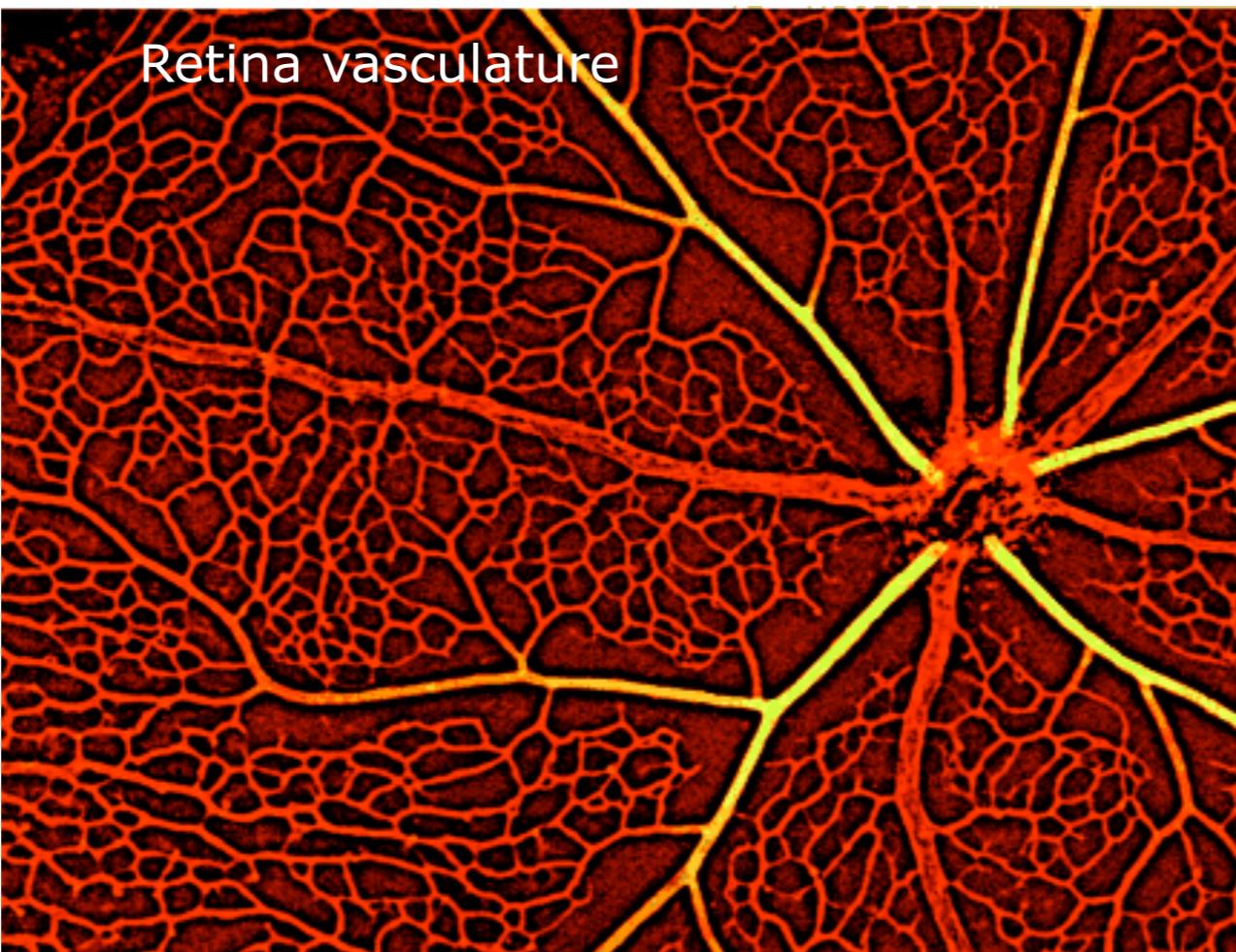


Canarium pulchrebracteatum

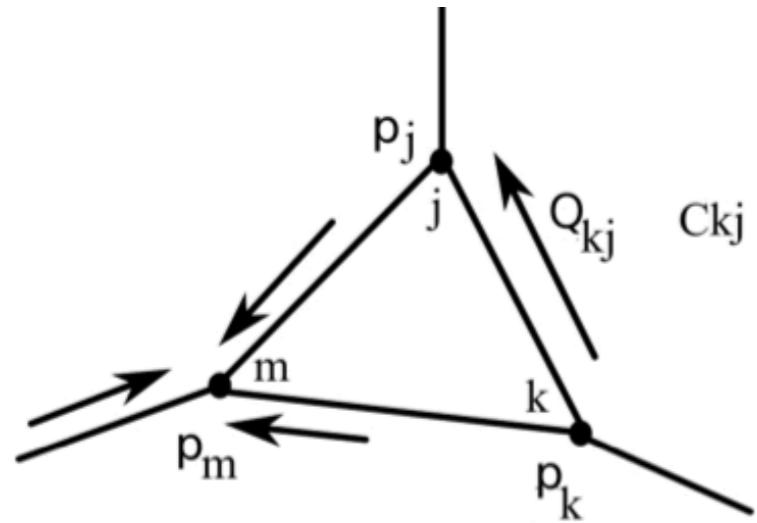


Biological transport systems

Fruttiger, IOVS (2002)



Adaptive update model



Laminar flow

Pairs of current sources and sinks

$$\sum_{j, \forall \{i,j\} \in \mathbb{E}} Q_{ij}^{kl} = \begin{cases} \zeta & : i = k \\ -\zeta & : i = l \\ 0 & : \text{else} \end{cases}$$
$$= (\delta_{ik} - \delta_{il}) \cdot \zeta.$$

Adaptive update model

Feedback term

$$\frac{dC_{ij}(t)}{dt} = \beta \cdot f\left(\frac{\langle |Q_{ij}(t)| \rangle}{\epsilon}\right) - \alpha \cdot C_{ij}(t)$$

use sigmoidal function for feedback term:

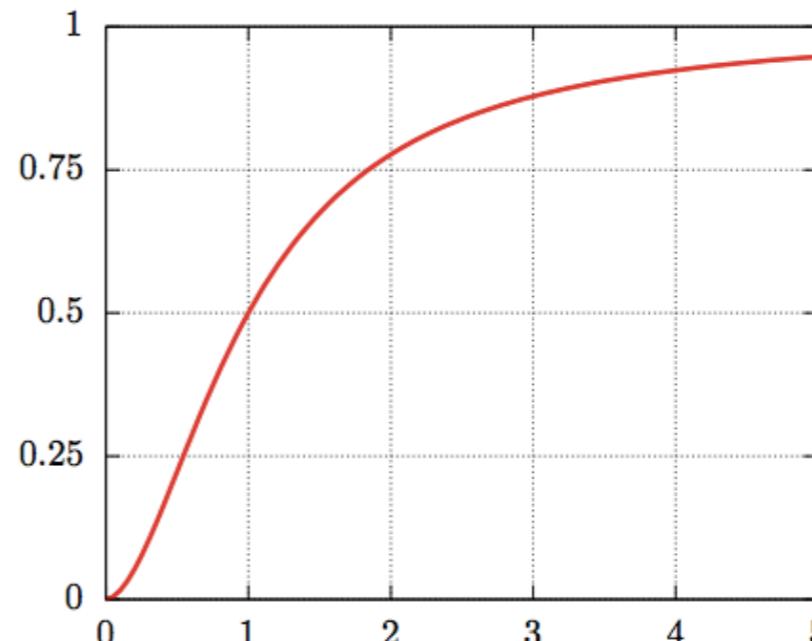
$$f(x) = \frac{x^\gamma}{1 + x^\gamma}$$

with $x := \frac{\langle |Q_{ij}(t)| \rangle}{\epsilon}$

features of feedback:

- no flow \Leftrightarrow no feedback
- positive
- limited

$f(x)$ for $\gamma = 1.8$

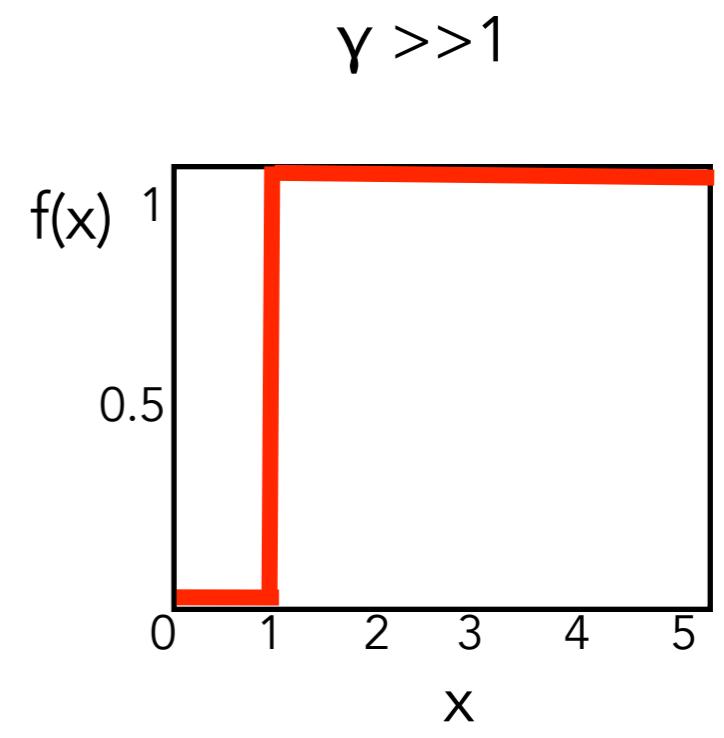
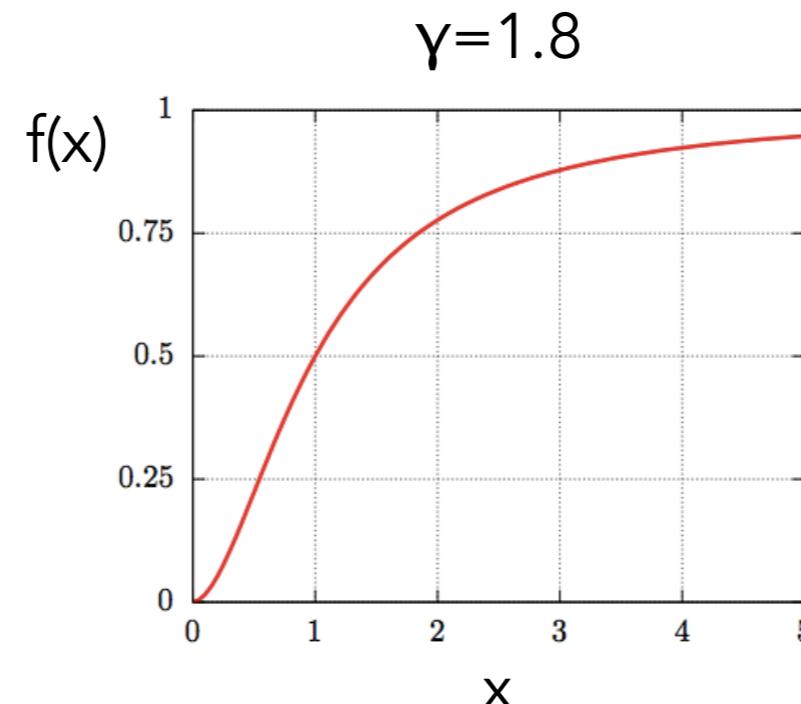
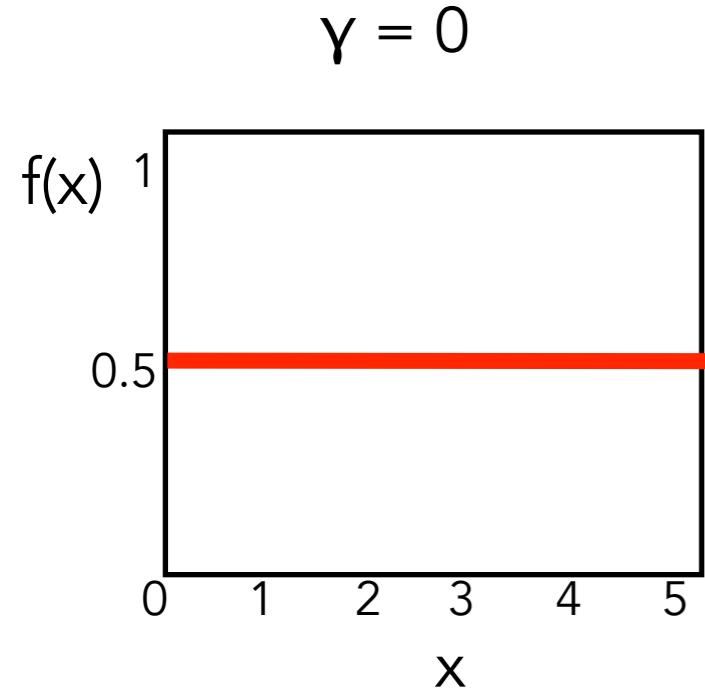


System depends on single dimensionless parameter: load $l_0 = \zeta/\epsilon$

Adaptive update model

$$\frac{dC_{ij}(t)}{dt} = \beta \cdot f\left(\frac{\langle |Q_{ij}(t)| \rangle}{\epsilon}\right) - \alpha \cdot C_{ij}(t)$$

Feedback term $f(x) = \frac{x^\gamma}{1 + x^\gamma}$



$C = \text{constant}$

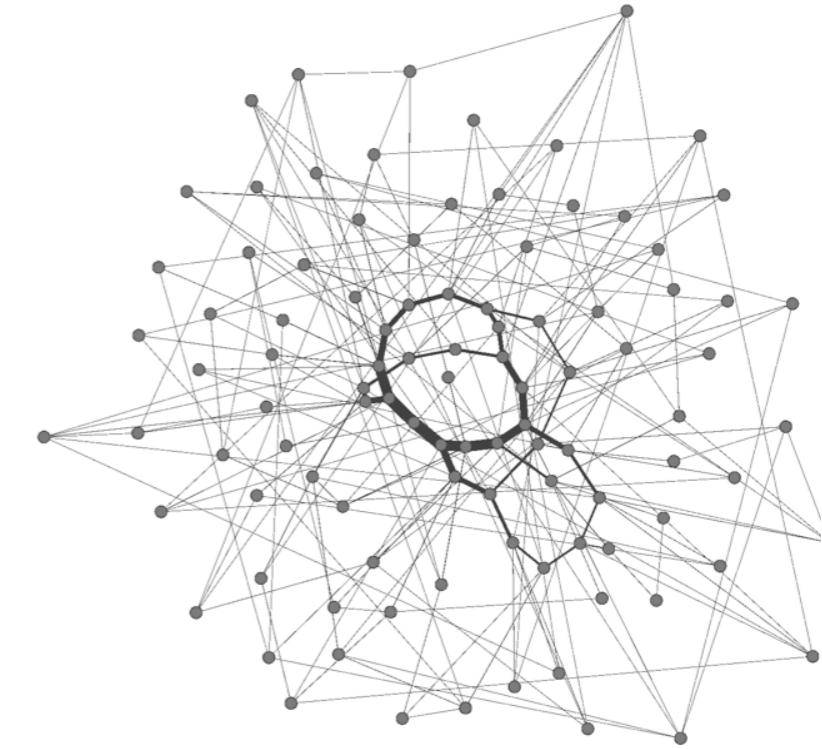
?

C bimodal

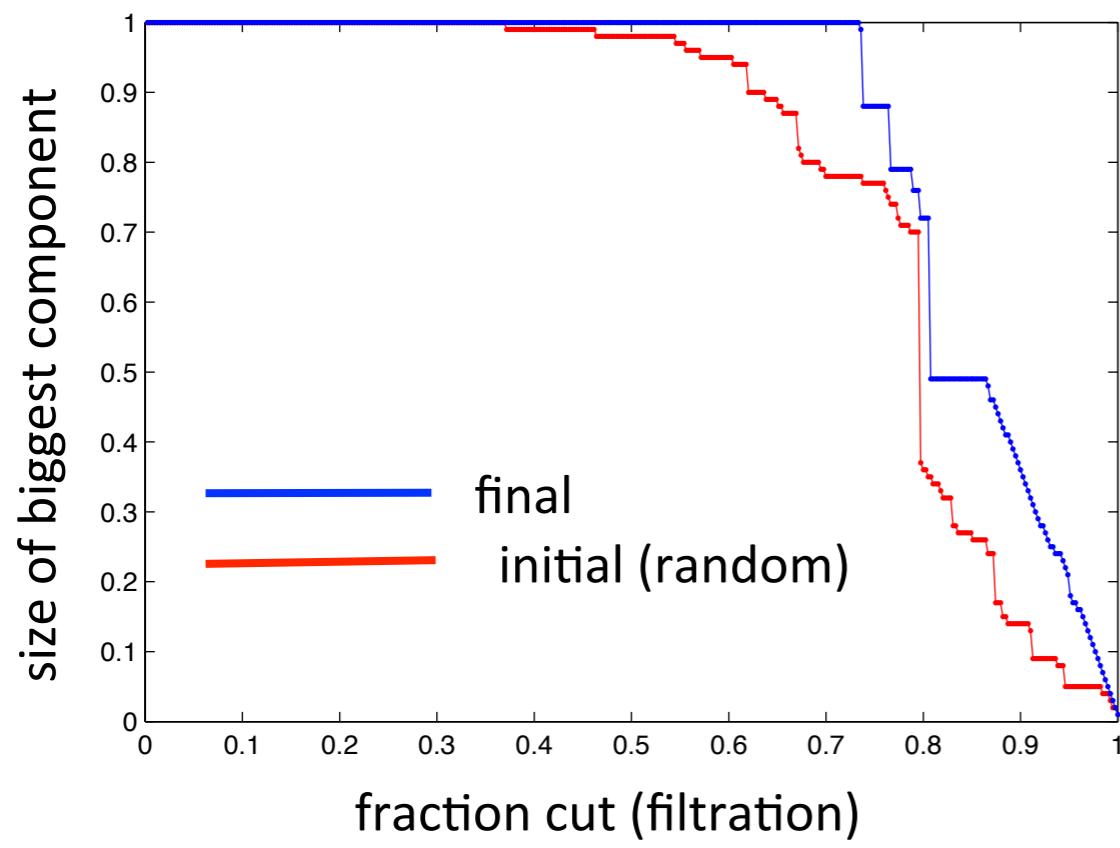
Which links non-zero?

Backbone formation

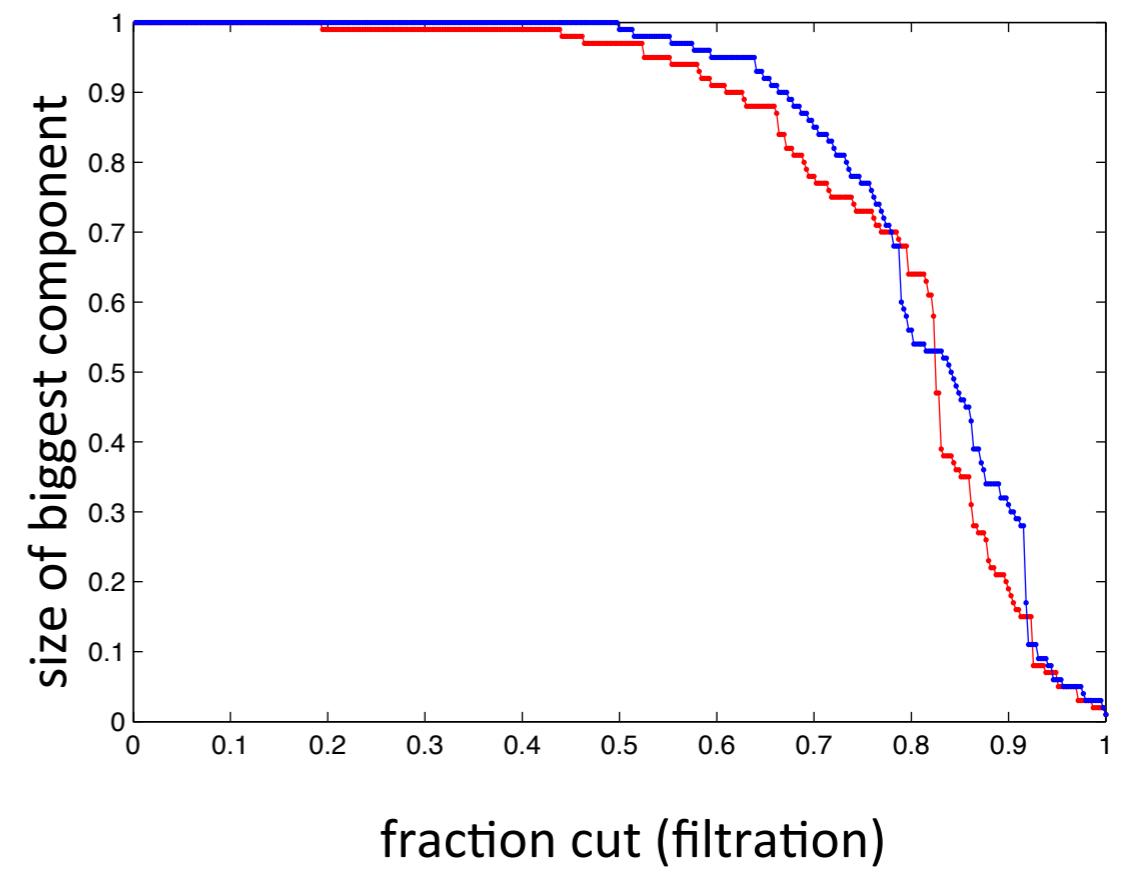
The loopy backbone increases the network robustness.



lo=1



lo=100



The group

Jana Lasser
(MSc)



Henrik Ronellenfitsch
(PhD)



Debshanka Manik
(PhD)



Johannes Gräwer
(PhD)



Jonathan Dawson
(Post-Doc)



Desislava Todorova
(Post-doc)

