Nonlinear time series analysis

Multivariate analysis

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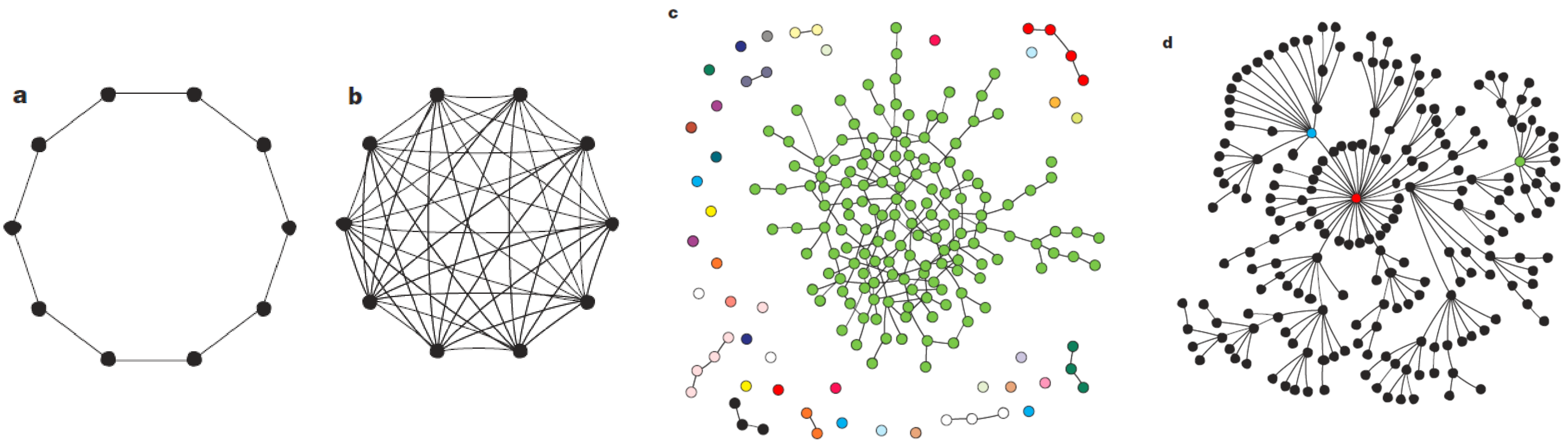
Outline

- **Introduction**
  - Historical developments: from dynamical systems to complex systems
- **Univariate analysis**
  - Methods to extract information from a time series.
  - Applications to climate data.
- **Bivariate analysis**
  - Extracting information from two time series.
  - Correlation, directionality and causality.
  - Applications to climate data.
- **Multivariate analysis**
  - Many time series: complex networks.
  - Network characterization and analysis.
  - Climate networks.

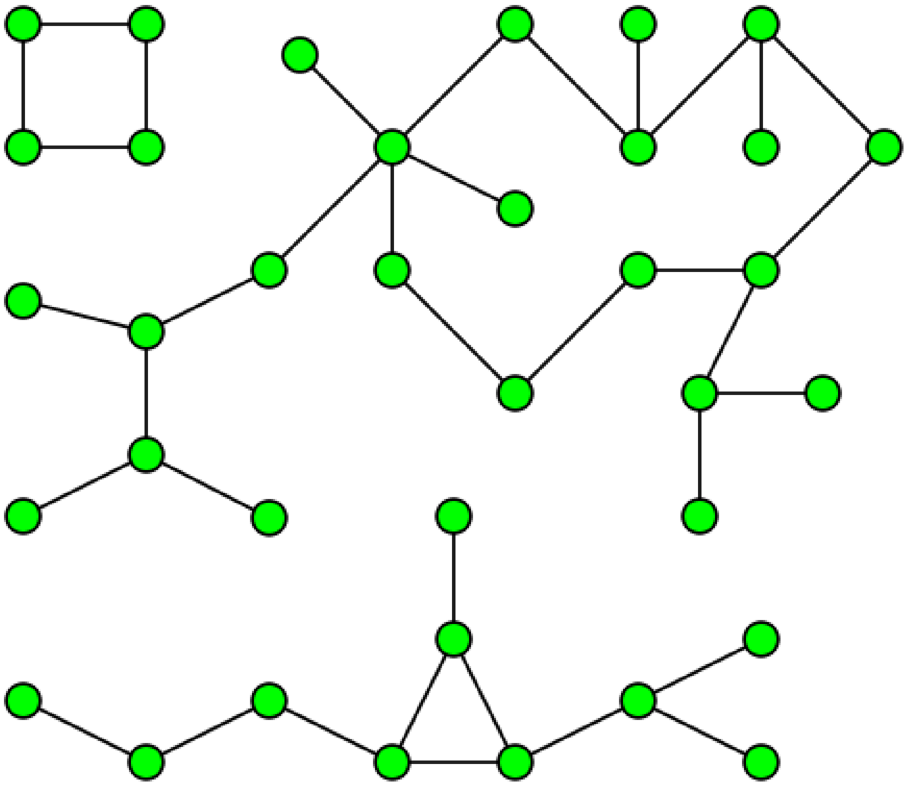
Networks or graphs

The challenge in the context of time series analysis: to infer the underlying network structure from observed signals.



Source: Strogatz
Nature 2001

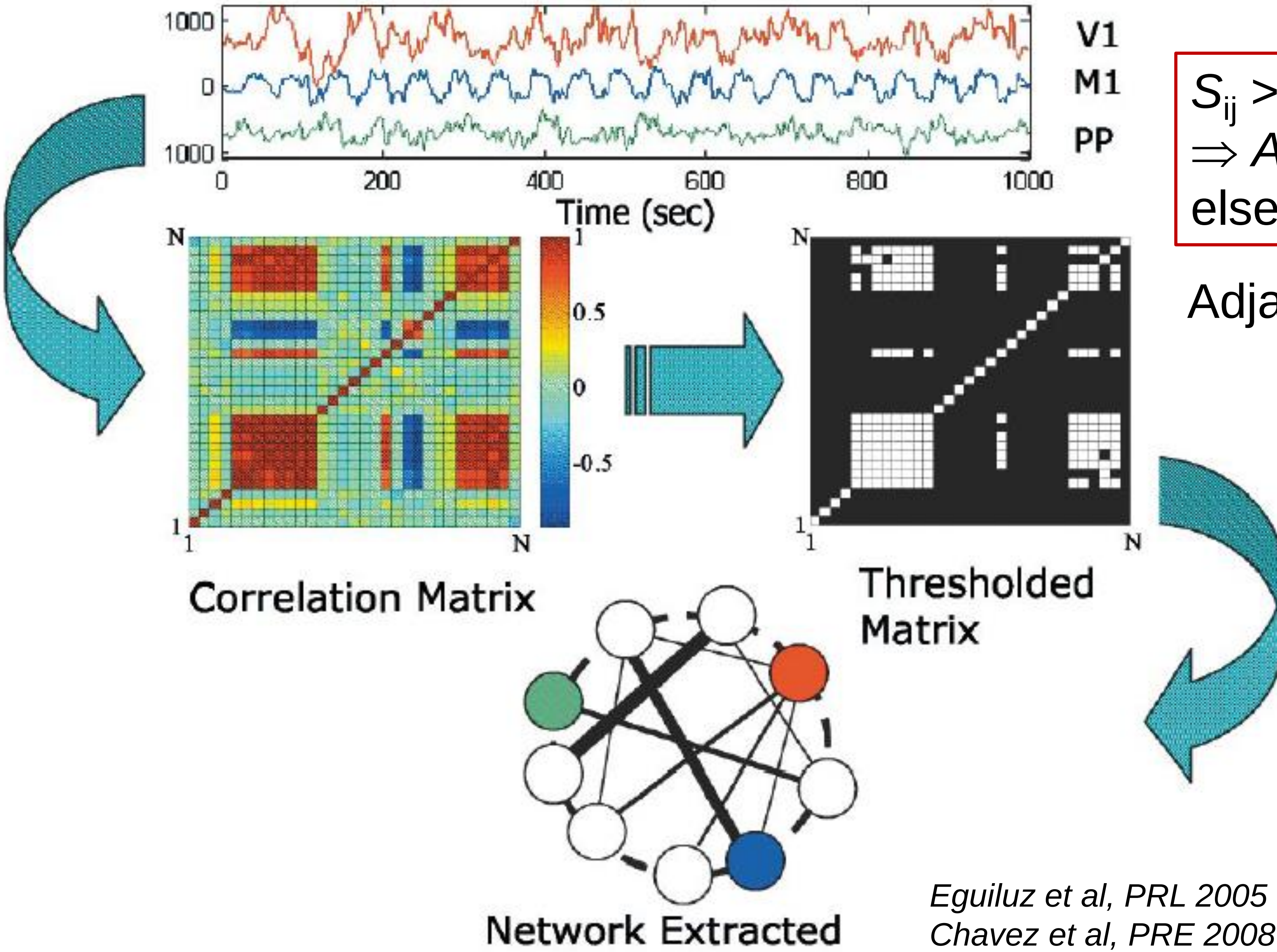
Connected components ("communities")



A graph with three connected components.
Source: Wikipedia

Using statistical similarity measures to infer interactions from data: “functional networks”

Brain functional network

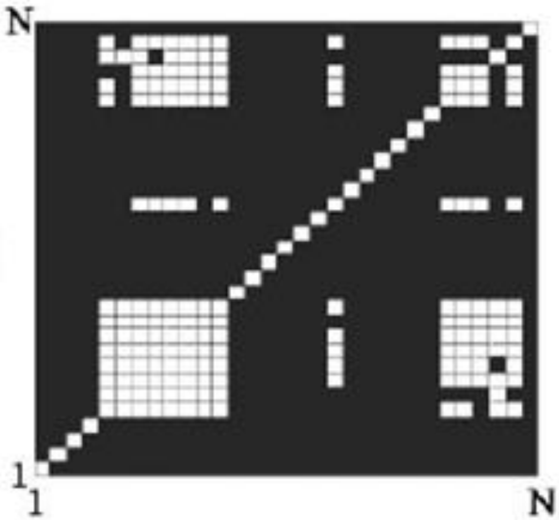


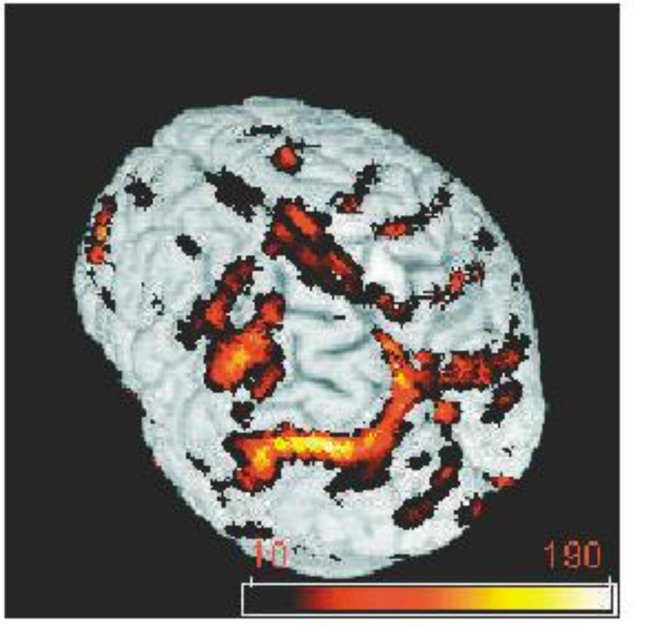
S_{ij} > Th
$\Rightarrow A_{ij} = 1$,
else A_{ij}=0

Adjacency
matrix

Eguiluz et al, PRL 2005
Chavez et al, PRE 2008

Graphical representation



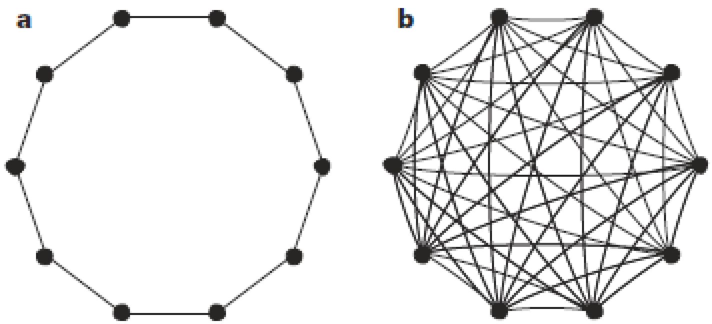


Thresholded matrix = inferred (“functional”) adjacency matrix

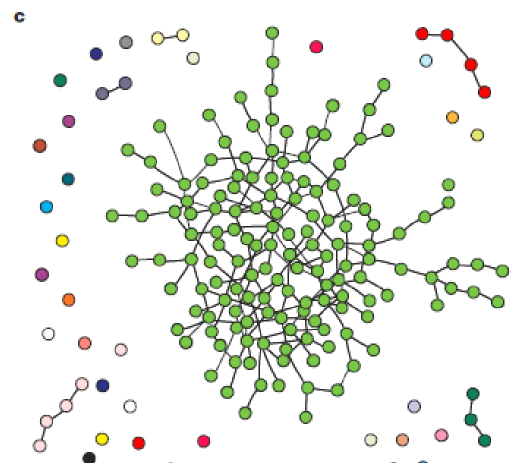
Degree of a node: number of links, $k_i = \Sigma_j A_{ij}$

The degree distribution: usual way to characterize a graph

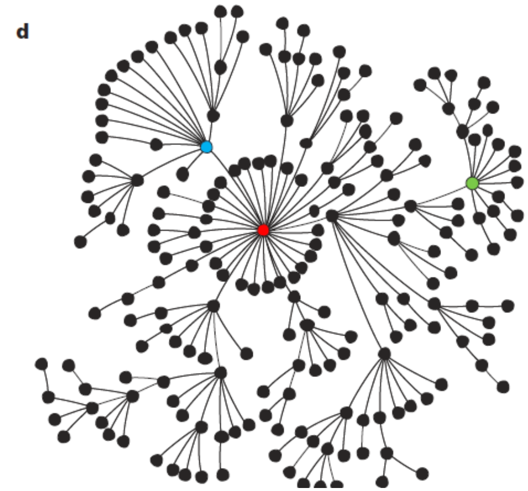
Regular

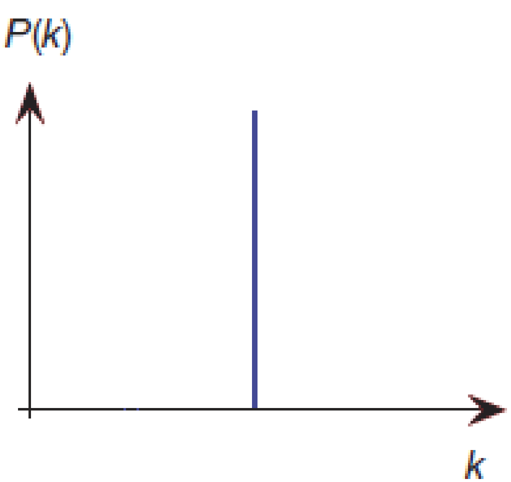


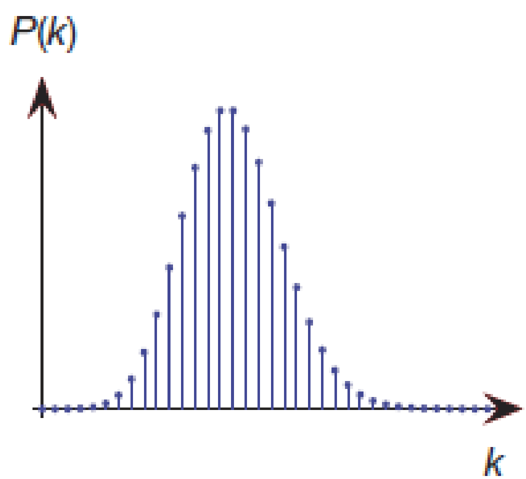
Random

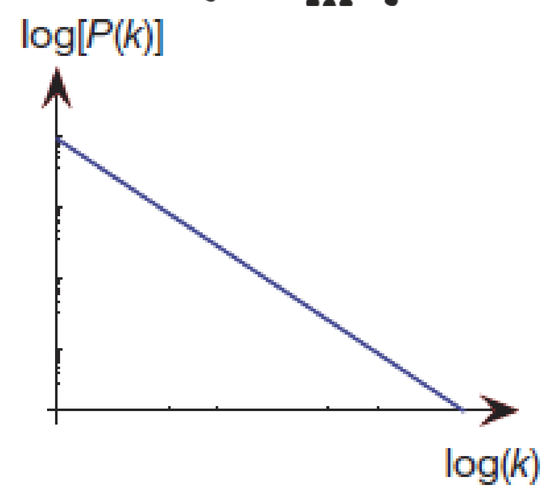


Scale-free



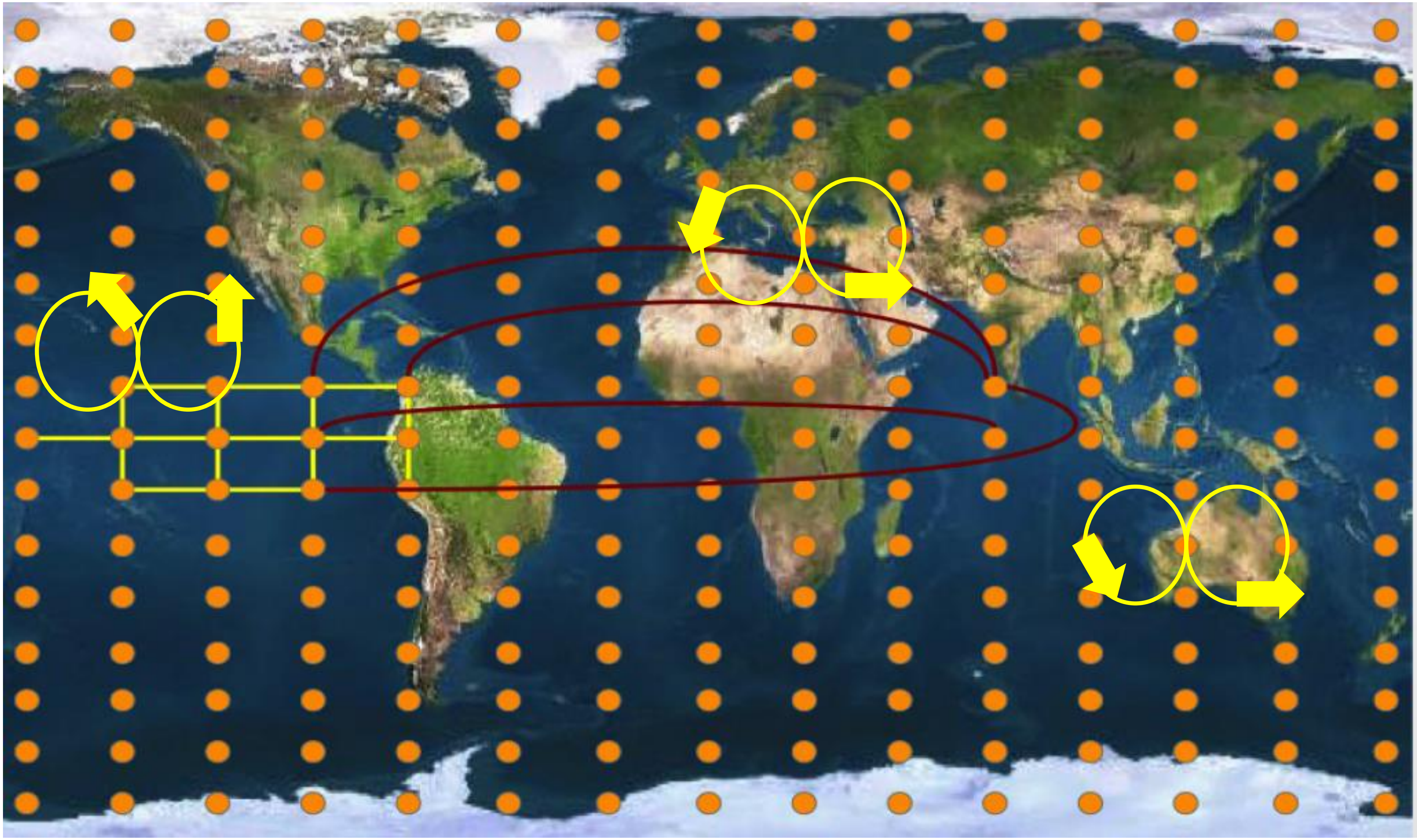




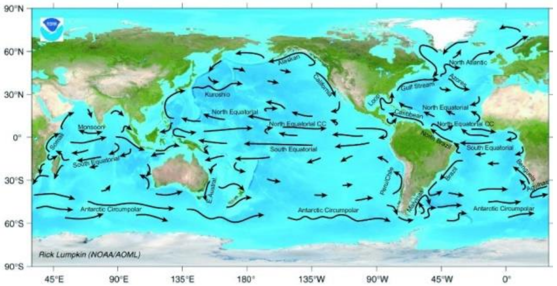


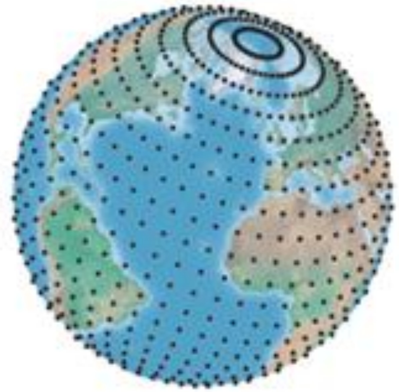
Strogatz, Nature 2001

The climate system as a set of “interacting oscillators”



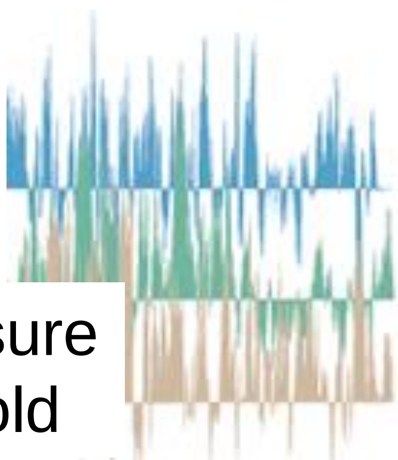
Complex network representation of the climate system





More than 10000 nodes (with different sizes).

Back to the climate system: interpretation (currents, winds, etc.)



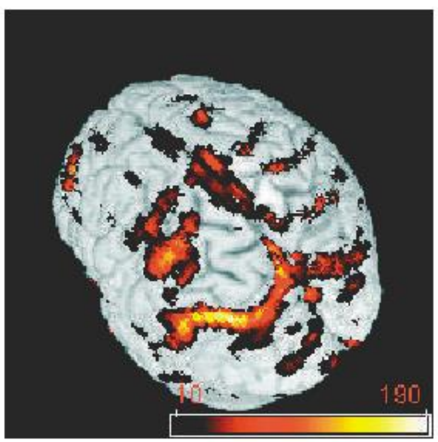
Daily resolution: more than 13000 data points in each TS

Sim. measure + threshold

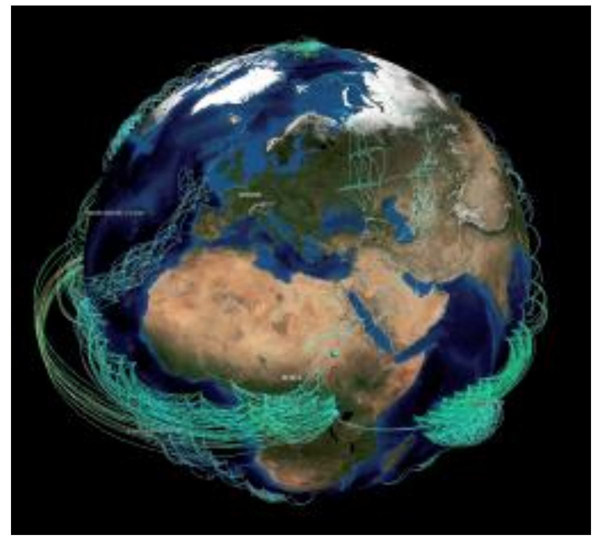
Surface Air Temperature
<u>Anomalies</u> (solar cycle removed)

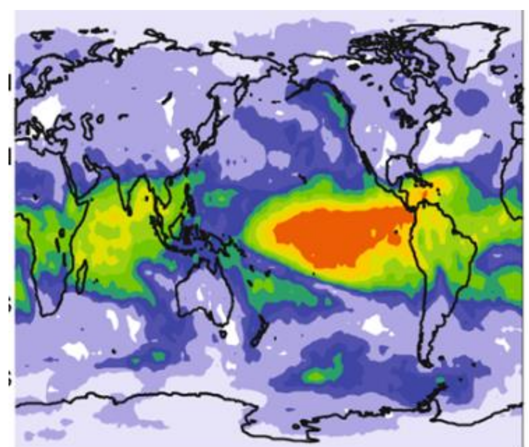
Donges et al, Chaos 2015

Brain network



Climate network





Area weighted connectivity (AWC): is the weighted degree (nodes are areas with different sizes)

$$\mathrm{AWC}_i = \frac{\sum_j^N A_{ij}\cos\left(\lambda_j\right)}{\sum_j^N \cos\left(\lambda_j\right)}$$

- Is the statistical similarity measure (S_{ij}) between the time series in two nodes (i,j) is "significant", the nodes are linked, otherwise, they are not.

$$\boxed{\begin{array}{l} S_{ij} > \mathrm{Th} \Rightarrow \\ A_{ij} = 1\text{, else} \\ A_{ij}=0 \end{array}}$$

How to select the threshold?

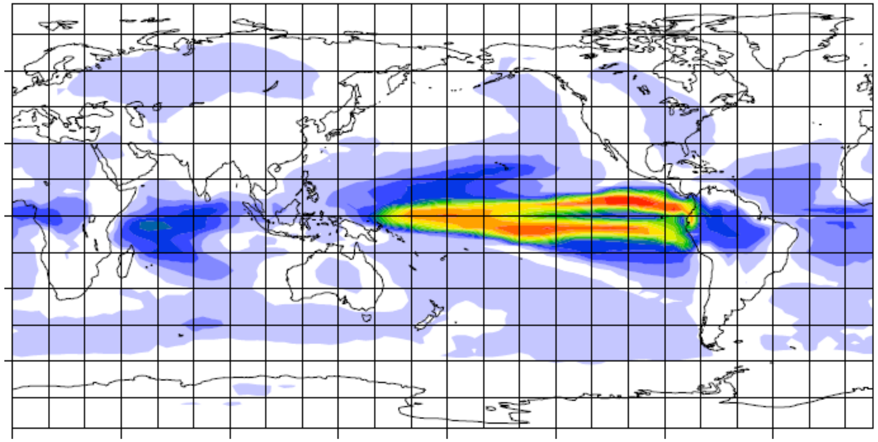
Three criteria are typically used:

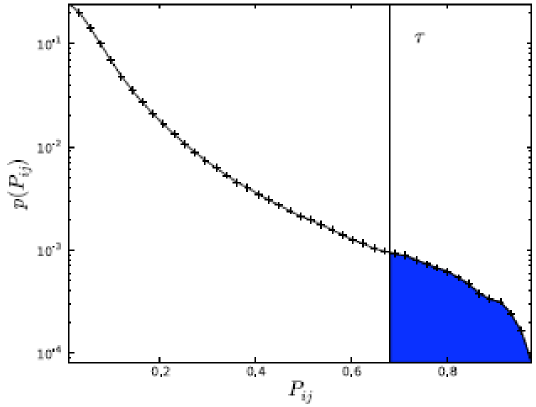
- A significance level is used (typically 5%) in order to omit connectivity values that can be expected by chance;
- We select an arbitrary value as threshold, such that it gives a certain pre-fixed number of links (or link density);
- We define the threshold as large as possible while guaranteeing that all nodes are connected (or a so-called “giant component” exists).

C. M. van Wijk et al., “*Comparing Brain Networks of Different Size and Connectivity Density Using Graph Theory*”, PLoS ONE 5, e13701 (2010)

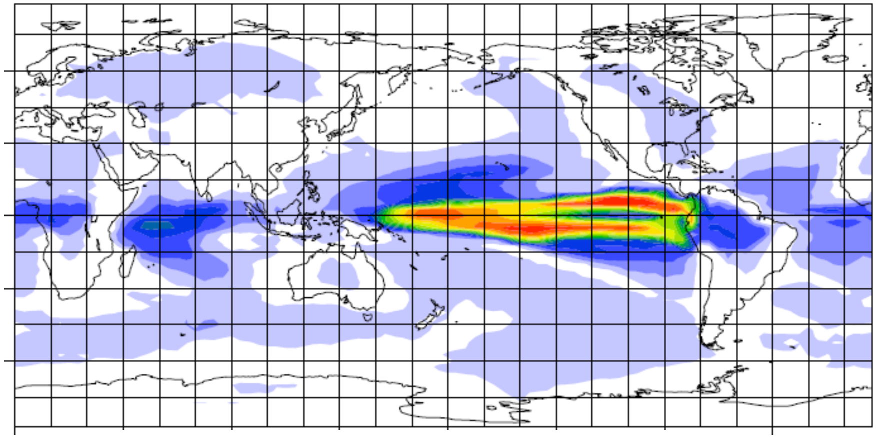
Comparison of area weighted connectivity with |CC| and MI

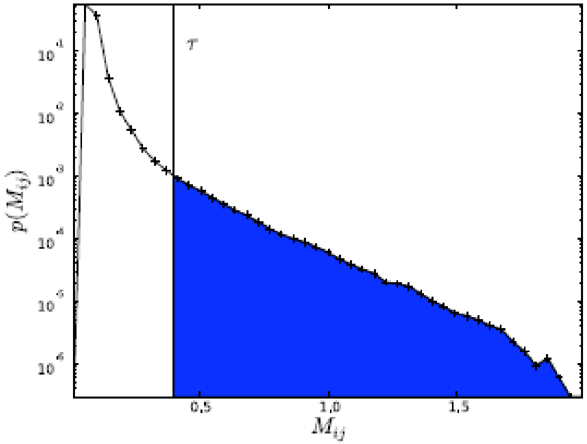
AWC computed with |cross-correlation|





AWC computed with mutual information



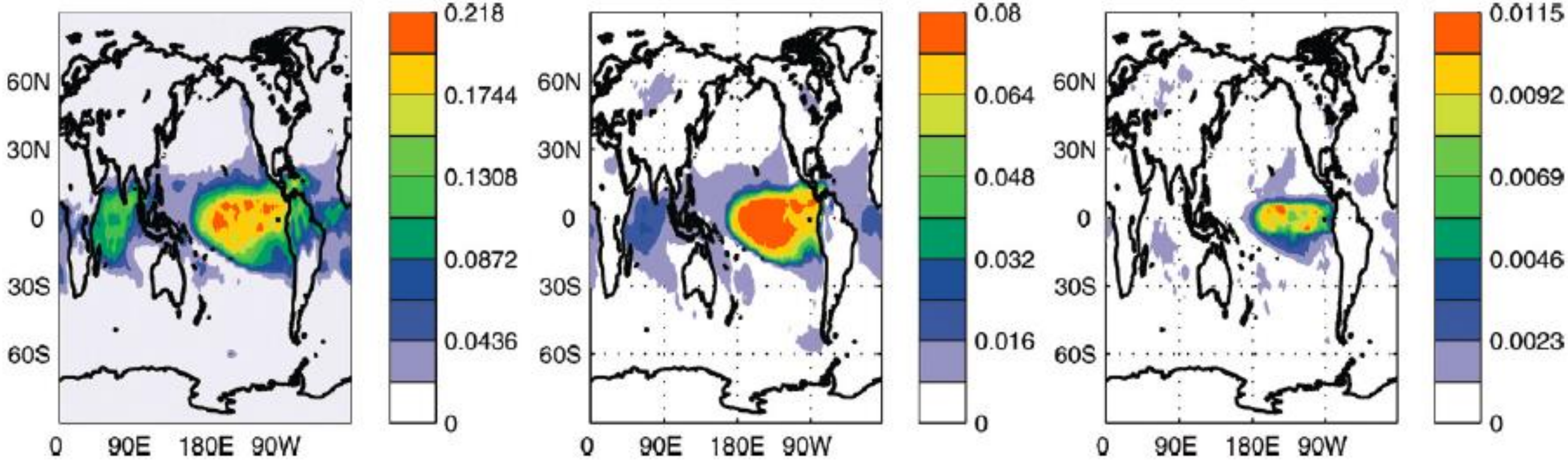


The threshold was selected to give a network with the same link density (0.005)

Donges et al, Eur. Phys. J. Special Topics 174, 157 (2009)

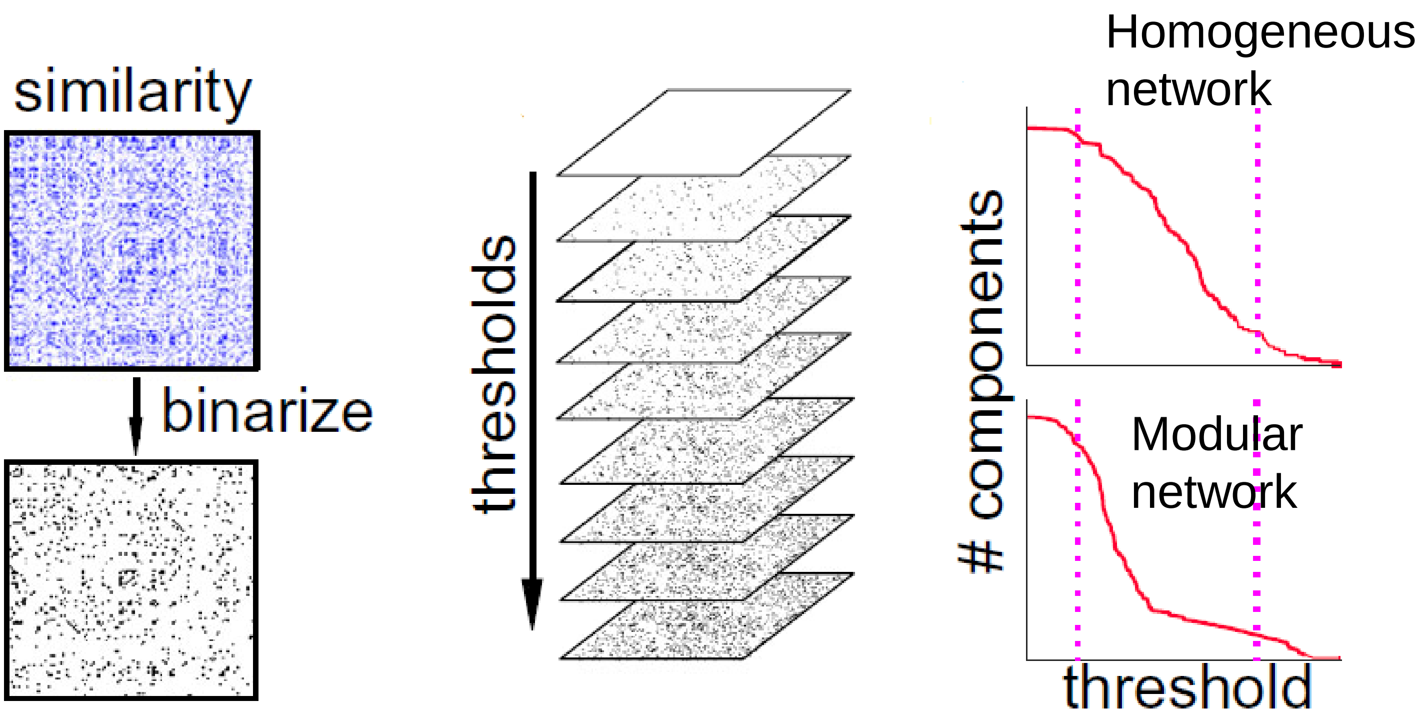
Influence of the threshold

$\rho=0.027$ $\rho=0.01$ $\rho=0.001$



M. Barreiro, et. al, Chaos 21, 013101 (2011)

Problems with thresholding



The number of *connected components* as a function of threshold reveals different structures.

- But thresholding near the dotted lines would suggest inaccurately that these two networks have similar structures.
- “Features” that persist for a wide range of thresholds are "true" features.

Giusti et al., J Comput Neurosci (2016) 41:1–14

Software

Unified functional network and nonlinear time series analysis for complex systems science: The pyunicorn package

Jonathan F. Donges' , Jobst Heitzig, Boyan Beronov, Marc Wiedermann, Jakob Runge, Qing Yi Feng, Liubov Tupikina, Veronika Stolbova, Reik V. Donner, Norbert Marwan, Henk A. Dijkstra, and Jürgen Kurths

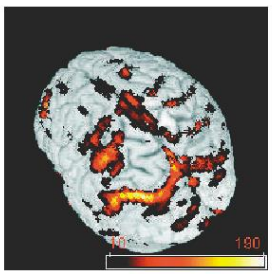
Citation: Chaos **25**, 113101 (2015); doi: 10.1063/1.4934554

View online: http://dx.doi.org/10.1063/1.4934554

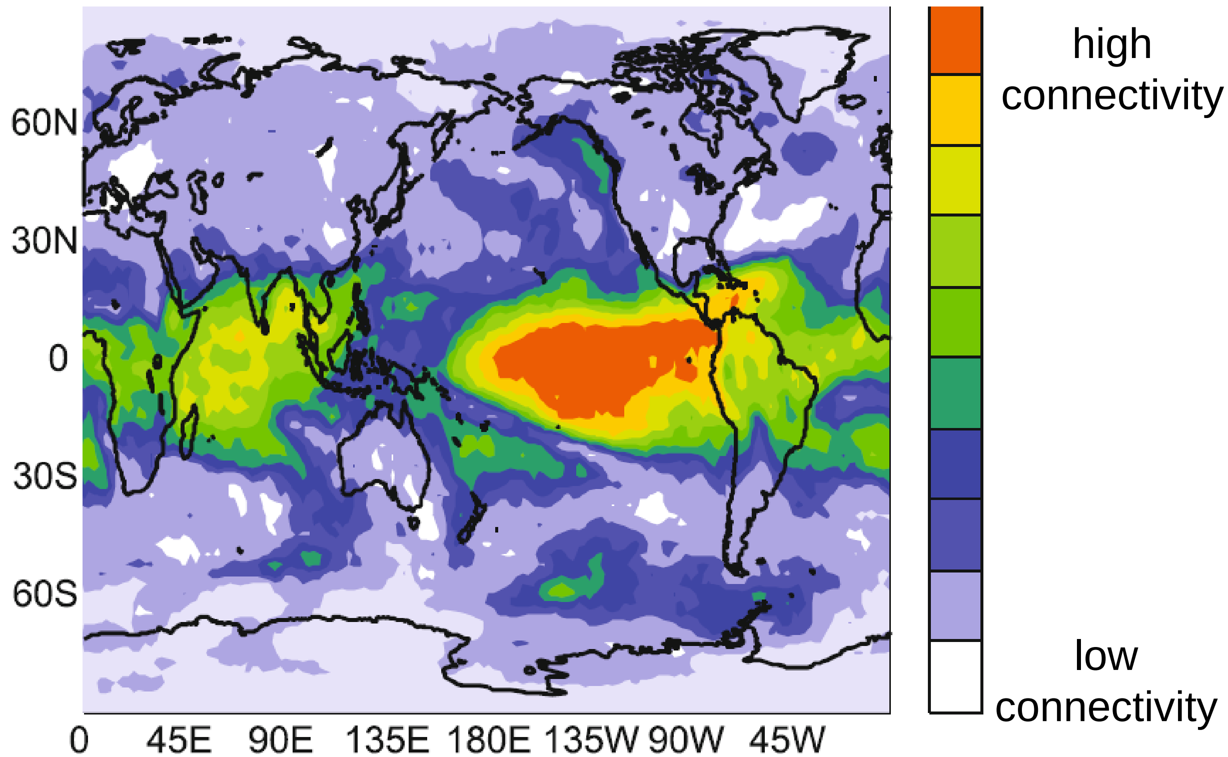
pyunicorn is available at https://github.com/pik-copan/

Climate network with mutual information computed with probabilities of ordinal patterns

$$\mathrm{AWC}_i = \frac{\sum_j^N A_{ij}\cos(\lambda_j)}{\sum_j^N \cos(\lambda_j)}$$



<u>inter-annual</u> time-scale (3 consecutive years). The color-code indicates the Area Weighted Connectivity (weighted degree)

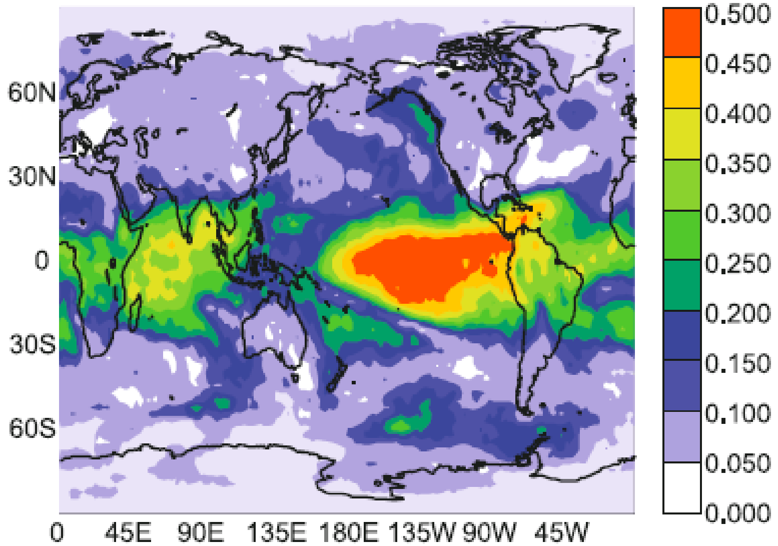


J. I. Deza, M. Barreiro, and C. Masoller, Eur. Phys. J. Special Topics 222, 511 (2013)

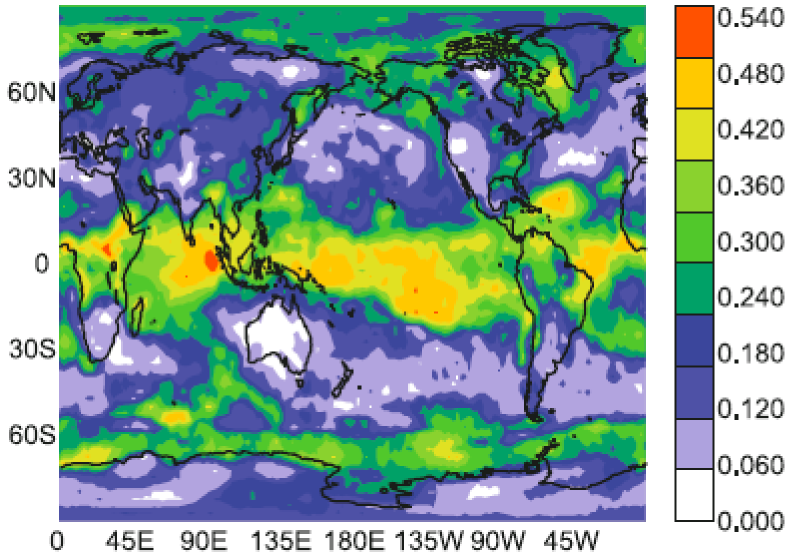
Comparison: ordinal probabilities vs. histogram of data values

$$M_{ij} = \sum_{m,n} p_{ij}(m,n) \log \frac{p_{ij}(m,n)}{p_i(m)p_j(n)}$$

Network when the probabilities are computed with ordinal analysis

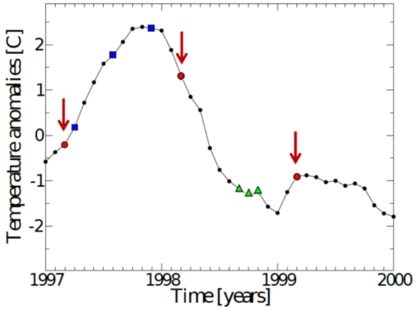


Network when the probabilities are computed with histogram of values



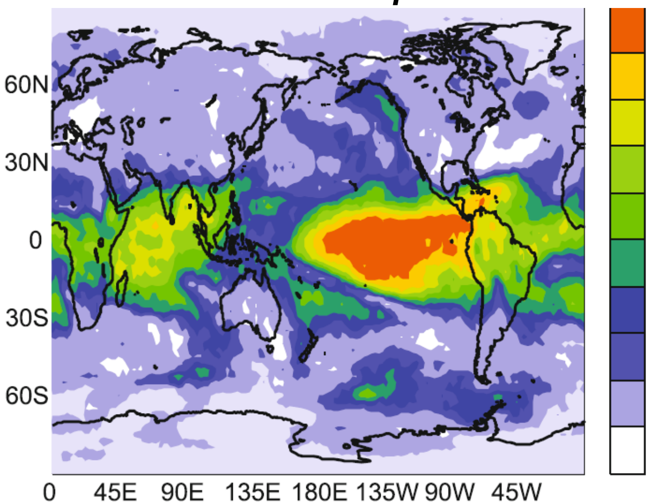
Color code indicates the area-weighted connectivity

inter-annual time scale

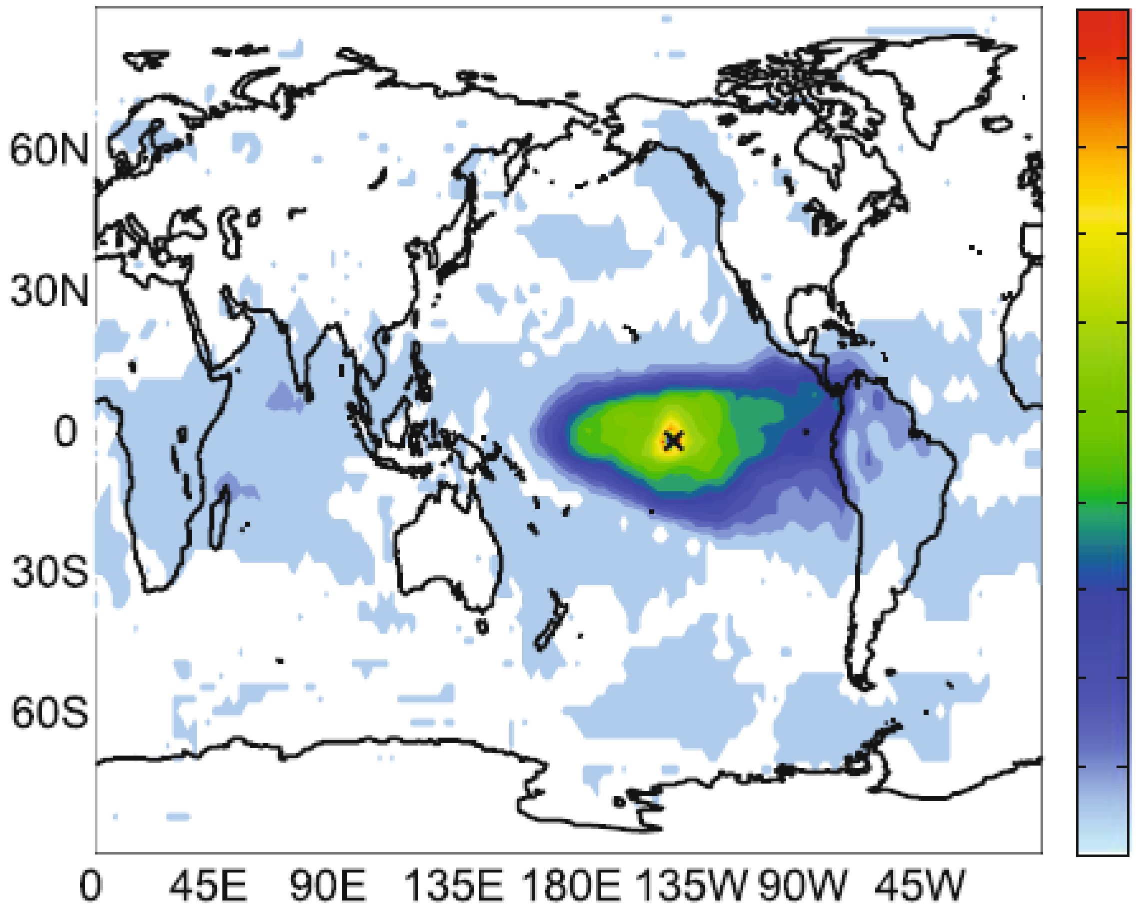


Who is connected to who?

AWC map



color-code indicates the MI values (only significant values)



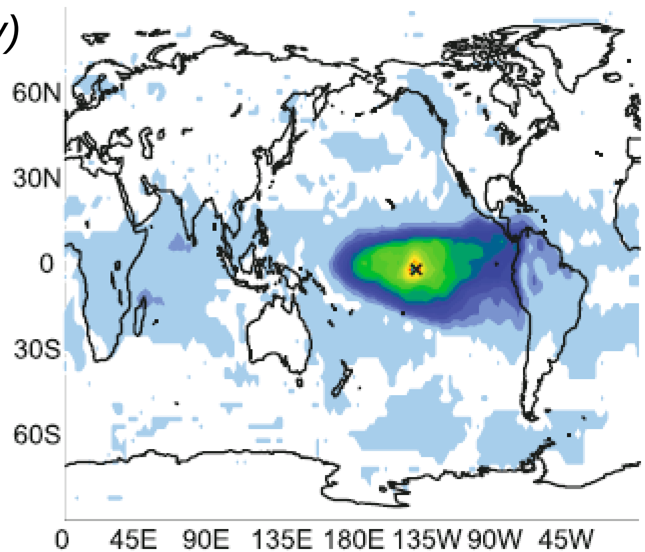
J. I. Deza, M. Barreiro, and C. Masoller, Eur. Phys. J. Special Topics 222, 511 (2013)

Influence of the threshold

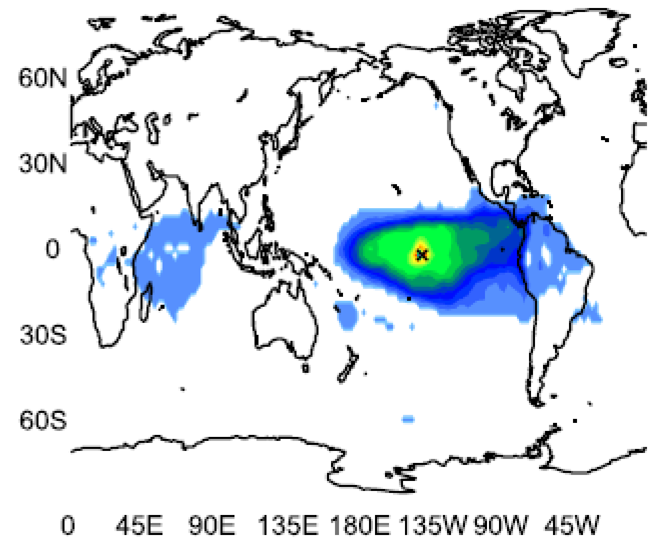
All significant links

(11% link density)

Color code: MI

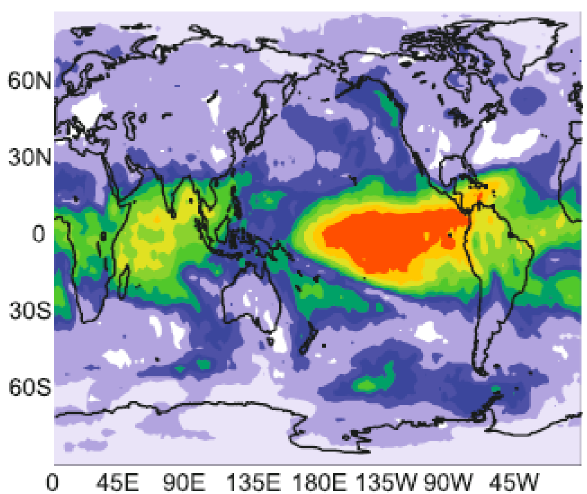


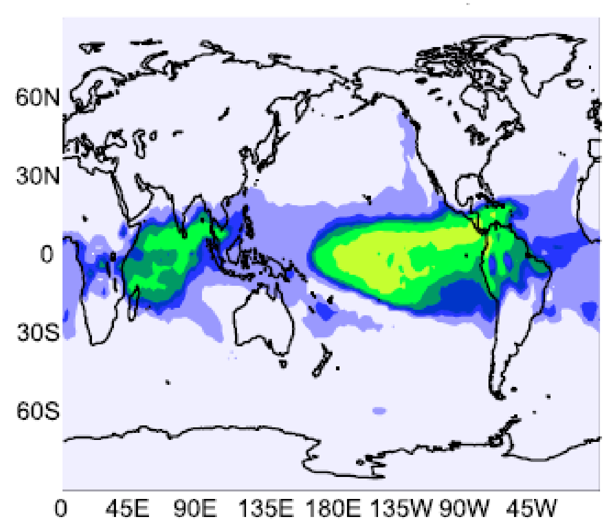
Higher threshold *(3% link density)*



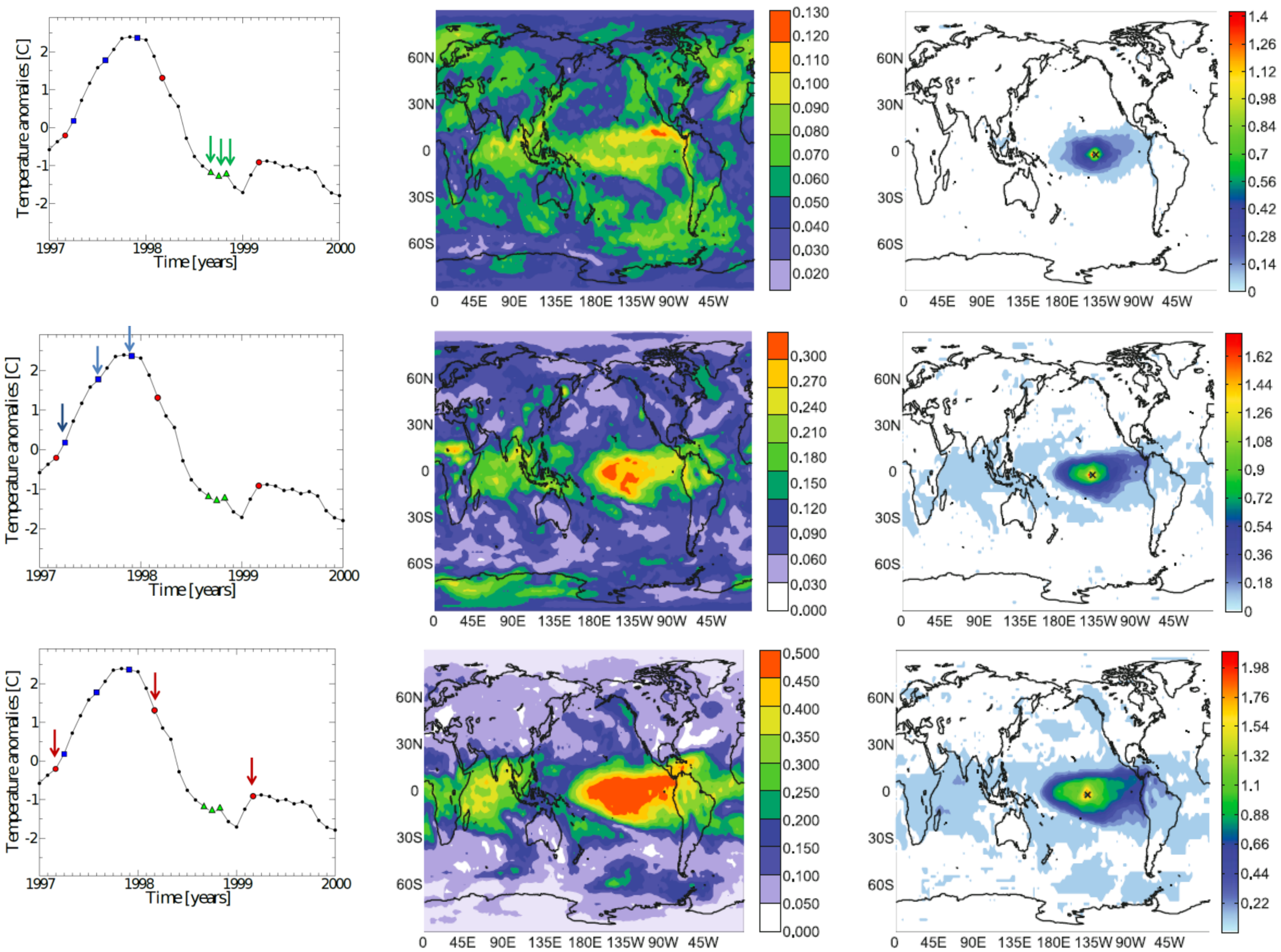
Color code: AWC

[Video]

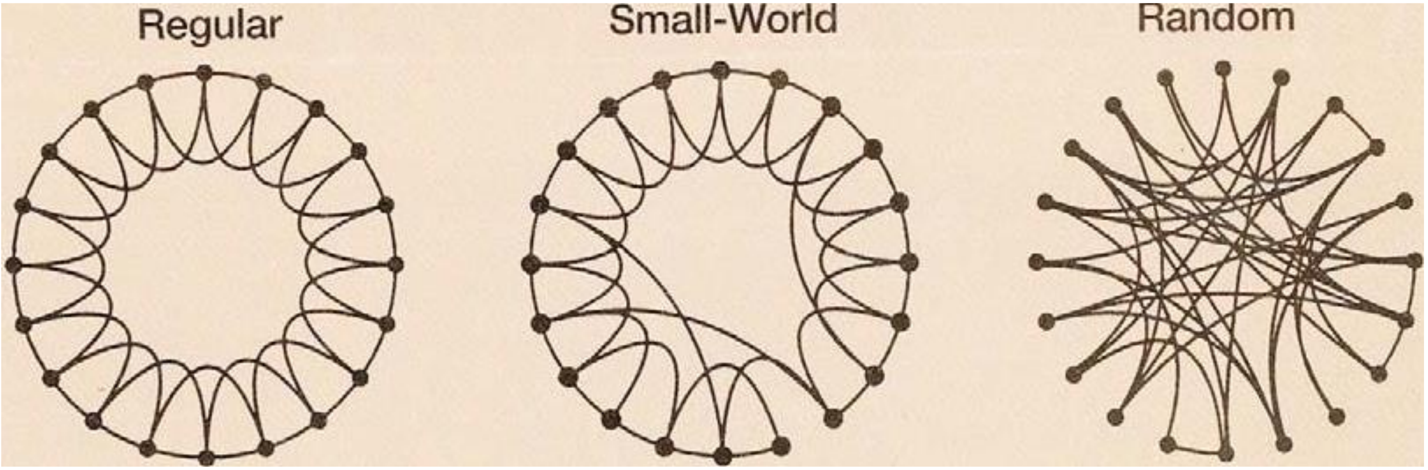




Influence of the time-scale of the pattern



Longer time-scale ⇒ increased connectivity



Network characterization

Definitions (for unweighted and undirected graphs)

- ***Adjacency matrix***: $A_{ij} = 1$ if i and j are connected, else $A_{ij} = 0$.

- ***Degree*** of a node $k_i = \Sigma_j A_{ij}$

- ***Clustering coefficient***: measures the fraction of a node's neighbors that are neighbors also among themselves

$$C_i = \frac{2R_i}{k_i(k_i-1)} = \frac{1}{k_i(k_i-1)} \sum_{j=1}^{N} \sum_{l=1}^{N} A_{ij} A_{jl} A_{li}$$

R_i is the number of connected pairs in the set of neighbors of node i

- ***Assortativity***: measures the tendency of a node with high/low degree to be connected to other nodes with high/low degree

$$a_i \equiv \frac{1}{k_i} \sum_{j=1}^{N} A_{ij} k_j$$

How to characterize the degree distribution?

- **Mean** (expected value of X): $\mu = \mathrm{E}[X] = \sum_{i=1}^{k} x_i\, p_i = x_1 p_1 + x_2 p_2 + \cdots + x_k p_k$

- **Variance**: $\sigma^2 = Var\ (X) = \mathrm{E}[(X-\mu)^2]$

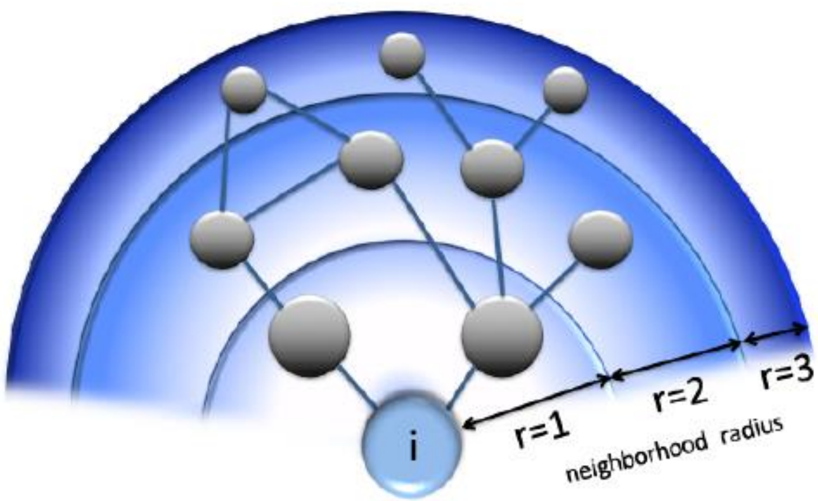
- **Skewness**: "measures" the asymmetry of the distribution

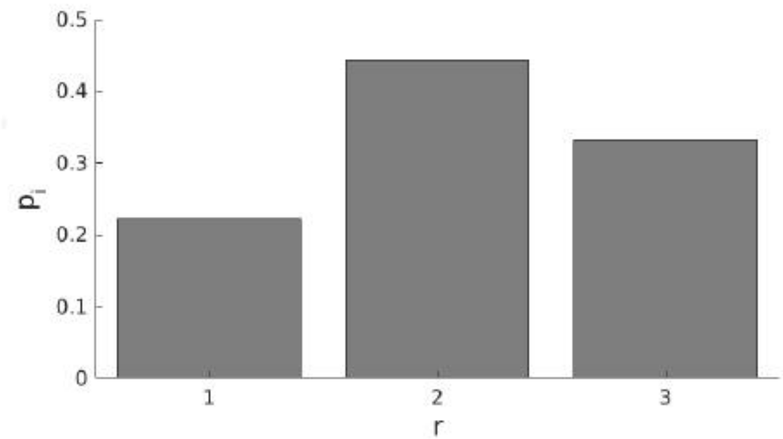
$$Z = \frac{X - \mu}{\sigma} \qquad S = \mathrm{E}[Z^3]$$

- **Kurtosis**: measures the "tailedness" of the distribution. For a normal distribution K=3.

$$K = \mathrm{E}[Z^4]$$

Diameter: longest shortest path





Node Distance Distribution (NDD) of node i: fraction of nodes that are connected to node i at distance j.

A. Viol et al Entropy **2019**, 21, 128

How to compare two distributions (degree, NDD, etc.)?

Distance between two distributions *P* and P_e

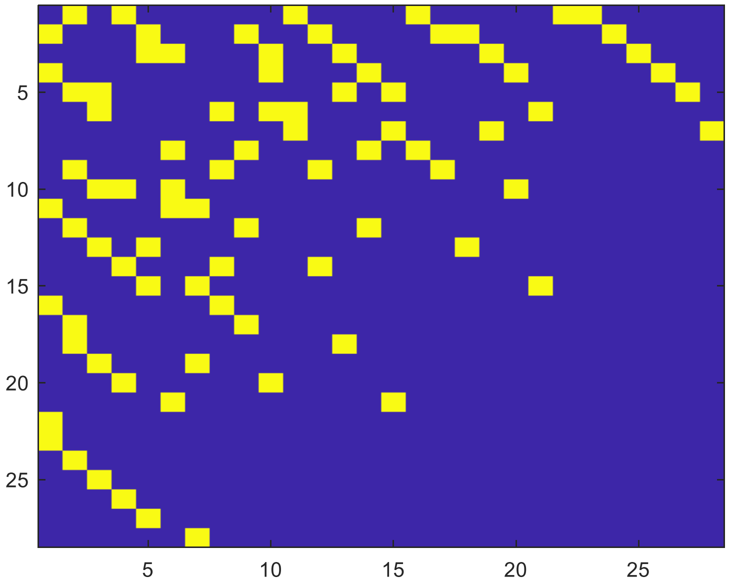
Euclidean $$D_E[P,P_e] = \left\| P - P_e \right\|_E = \sum_i \left(p_i - p_{i,e} \right)^2$$

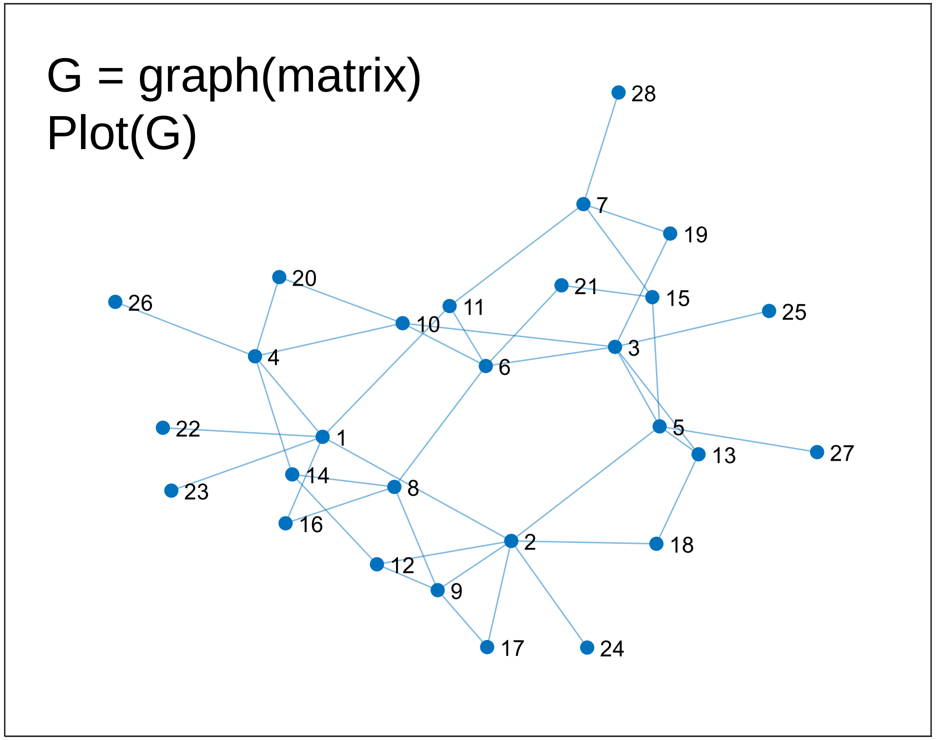
Kullback $$D_K[P,P_e] = K[P|P_e] = I\left[P_e\right] - I\left[P\right]$$

Jensen divergence $$D_J[P,P_e] = \frac{K\left[P|P_e\right] + K\left[P_e|P\right]}{2}$$

Read more: S-H Cha: *Comprehensive Survey on Distance/Similarity Measures between Probability Density Functions*, Int. J of. Math. Models and Meth. 1, 300 (2007)

Exercise 1: graphical representation of the “structural” network of the electronic circuits and calculate the degree distribution

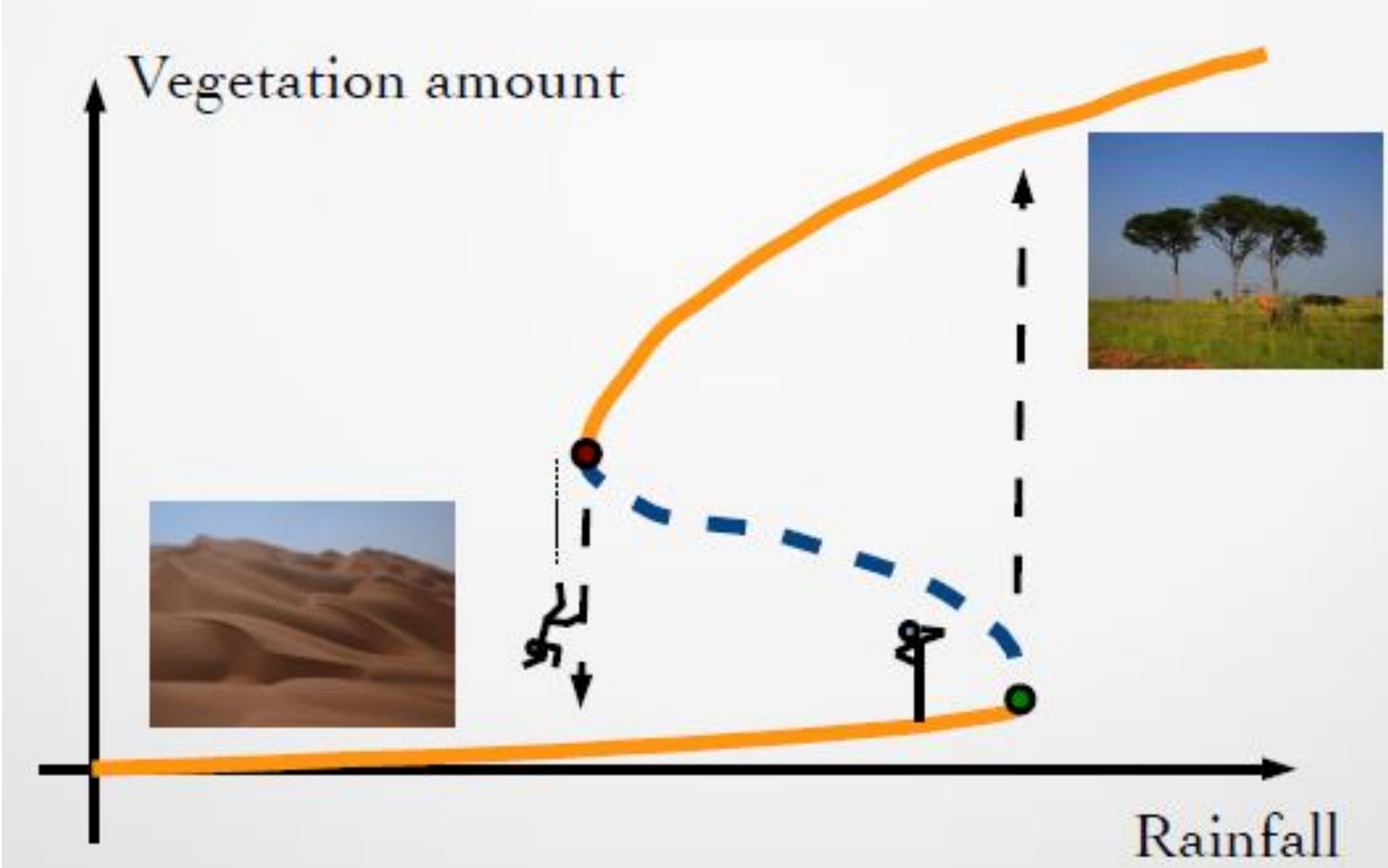




Exercise 2: analyze the functional network of the 28 electronic circuits

- Construct the network using the Pearson coefficient as statistical similarity measure.
- Calculate the mean degree for different values of the coupling for fixed TH.
- Calculate the mean degree for different values of the threshold for fixed coupling.

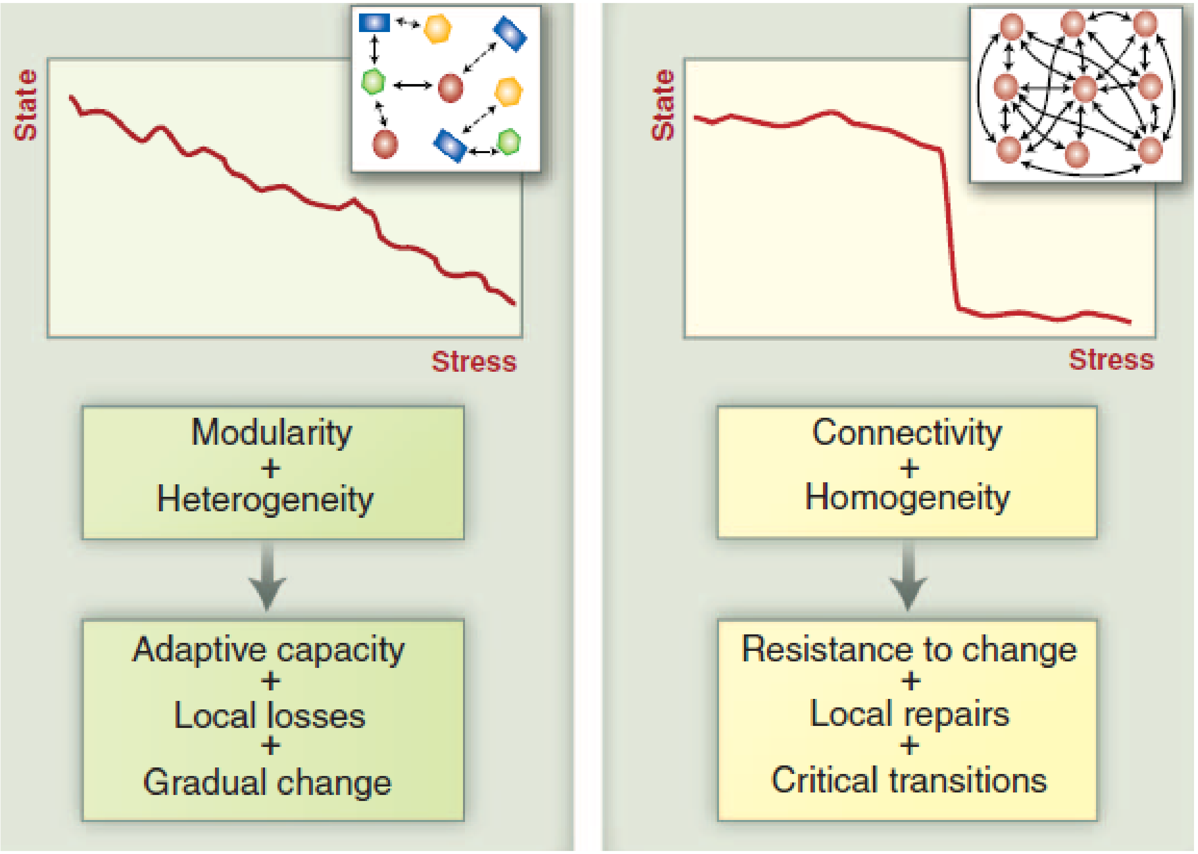
Example:
desertification transition under the lens of network analysis



Our goal: to develop reliable early-warning indicators

Can we use “correlation networks” to detect the approach to a tipping point?

Role of the network structure



Networks in which the components are heterogeneous and where incomplete connectivity causes modularity tend to gradually adjust to change.

In highly connected networks, local losses tend to be "repaired" by subsidiary inputs from linked units until at a critical stress level the system collapses.

Scheffer et al. Science 338, 344 (2012)

Desertification transition: model

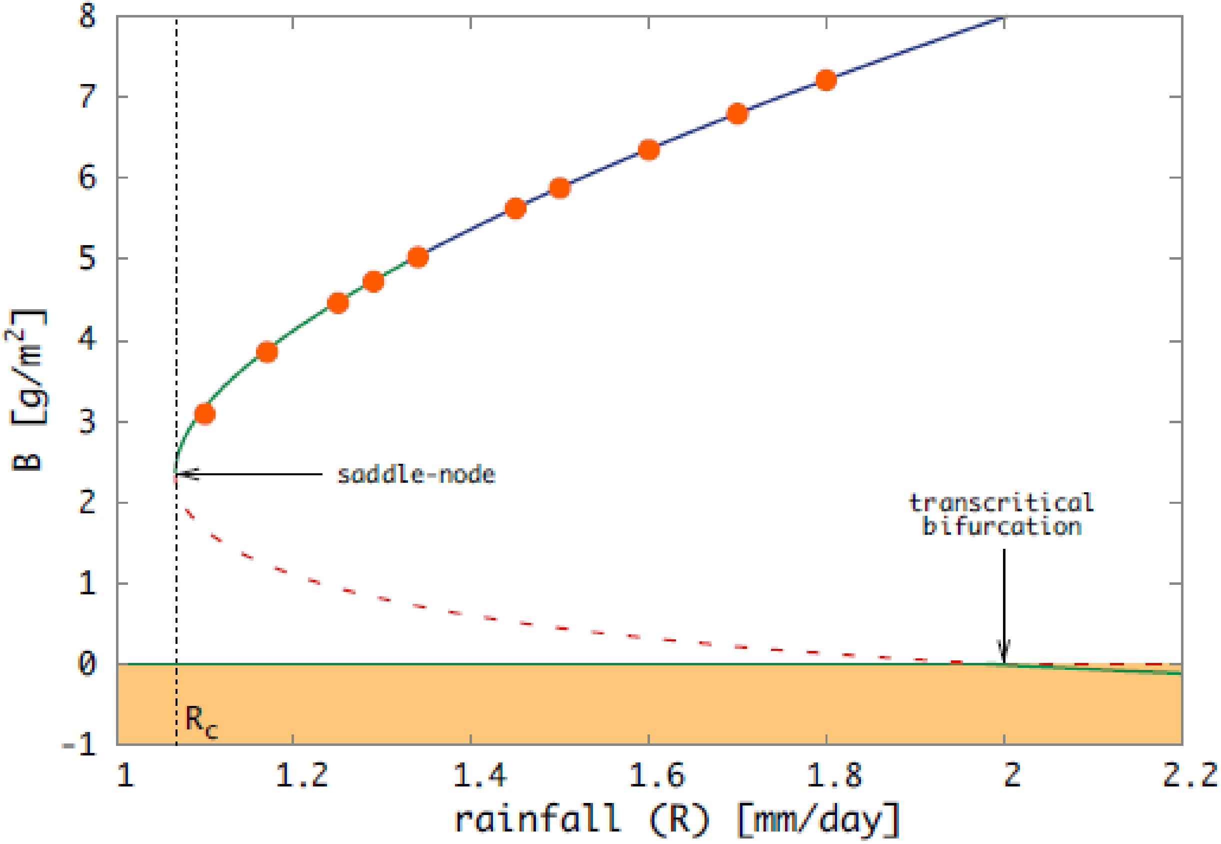
$$\frac{\partial w}{\partial t} = R - \frac{w}{\tau_w} - \Lambda w B + D\nabla^2 w + \sigma_w w_0 \xi^w(t),$$

$$\frac{\partial B}{\partial t} = \rho B\left(\frac{w}{w_0} - \frac{B}{B_c}\right) - \mu \frac{B}{B + B_0} + D\nabla^2 B + \sigma_B B_0 \xi^B(t)$$

- *w* (in mm) is the soil water amount
- *B* (in g/m^2) is the vegetation biomass
- Uncorrelated Gaussian white noise
- *R* (rainfall) is the bifurcation parameter

Shnerb et al. (2003), Guttal & Jayaprakash (2007), Dakos et al. (2011)

Saddle-node bifurcation

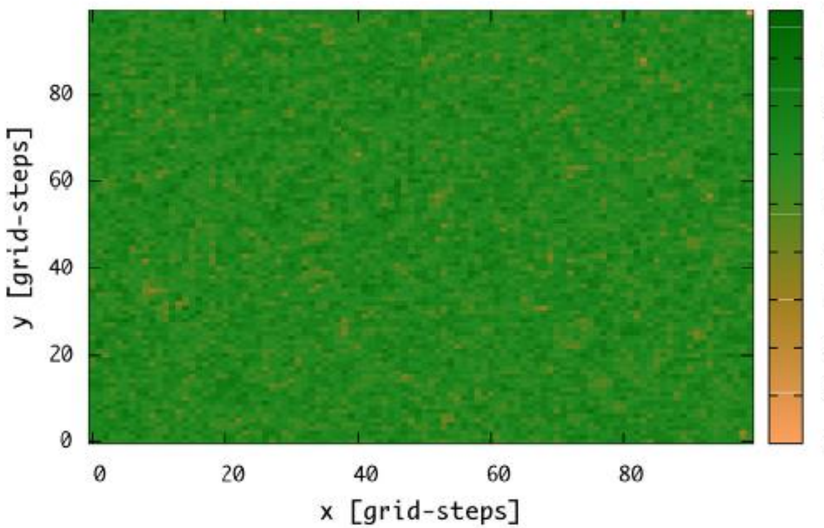


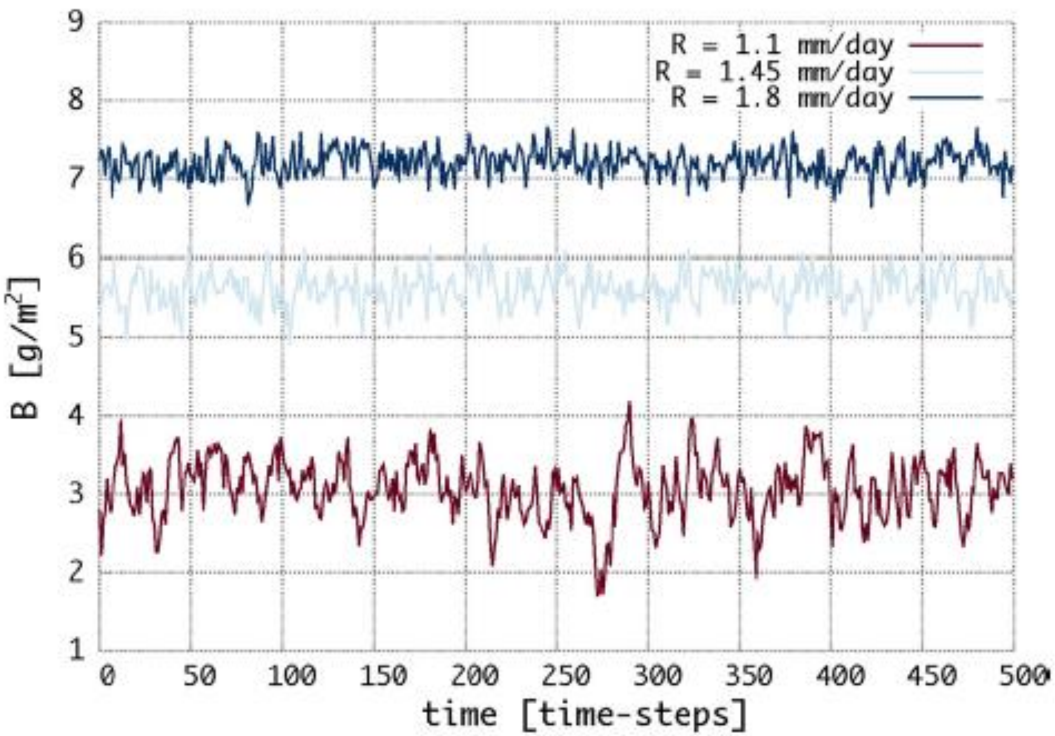
$R<R_c$: only desert-like solution (B=0)

R_c = 1.067 mm/day

Biomass time series

Biomass B when R=1.1 mm/day





100 m x 100 m = 10^4 grid cells
Simulation time 5 days in 500 time steps
Periodic boundary conditions

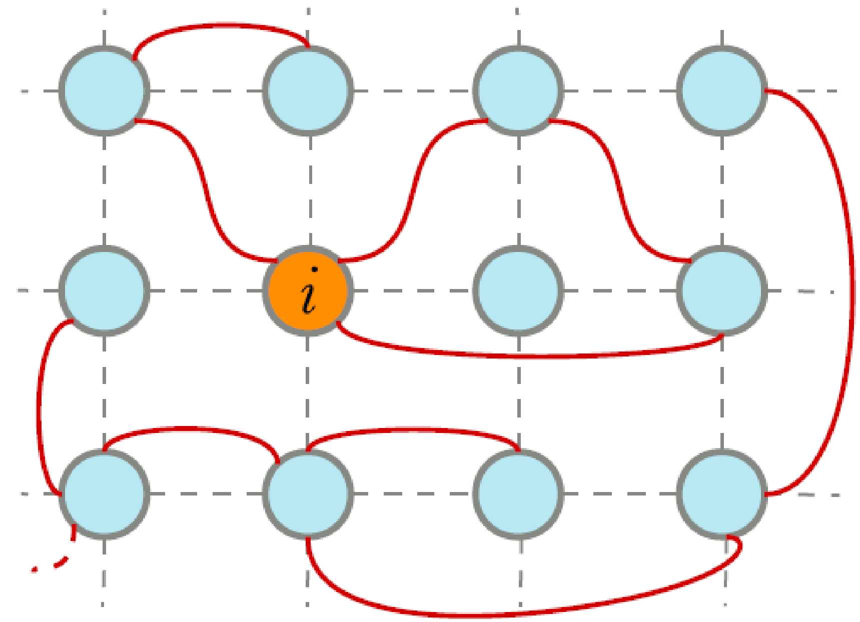
Correlation Network

$S_{ij} > Th \Rightarrow A_{ij} = 1$, else $A_{ij}=0$

A_{ij} is the adjacency matrix

Statistical similarity measure: Pearson coef.= |zero-lag cross-correlation|

Threshold: $Th=0.2$ keeps only significant correlations ($p<0.05$)



G. Tirabassi et al., Ecological Complexity (2014)

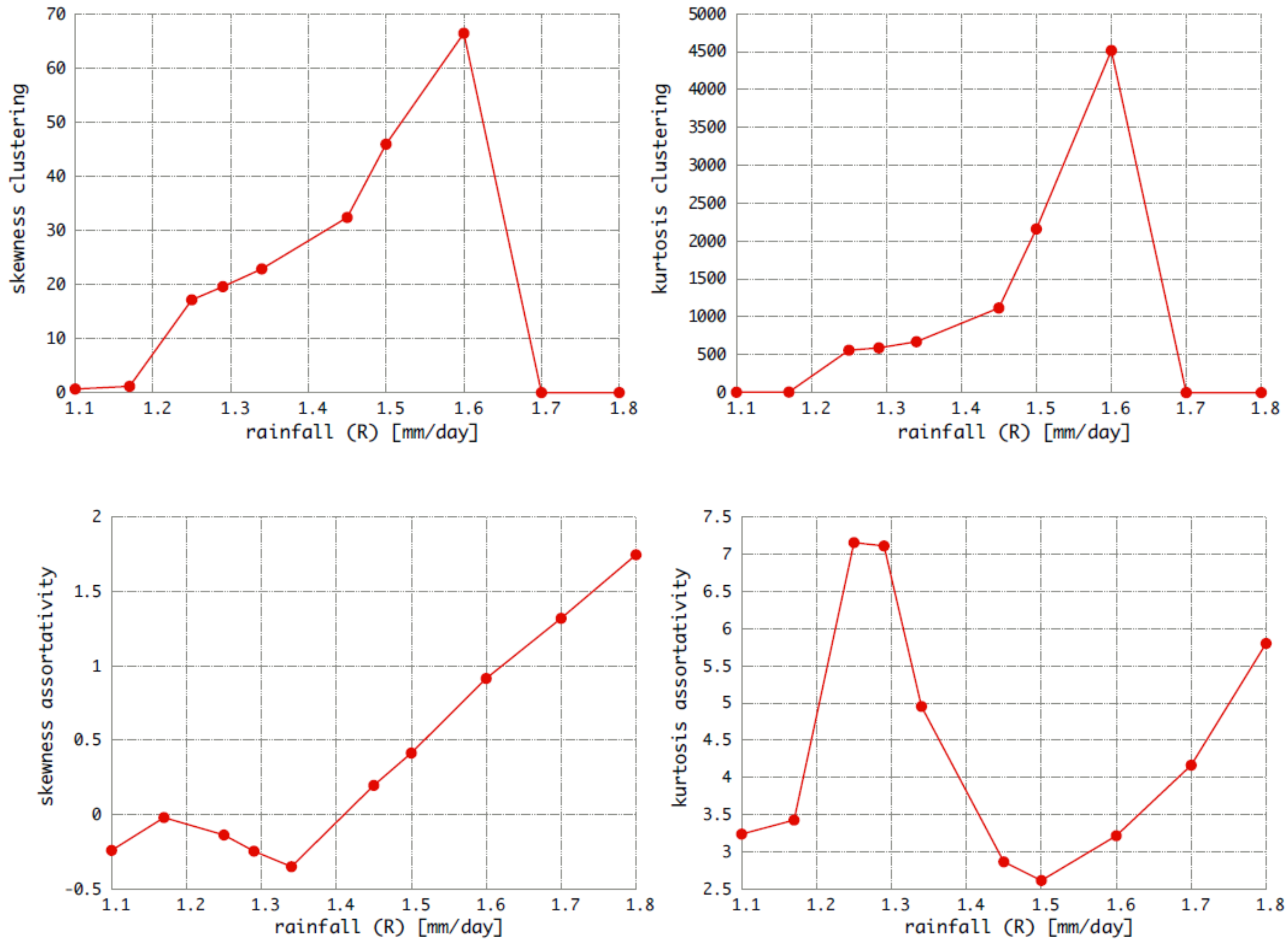
“Randomization” of the correlation network as the tipping point is approached

skewness

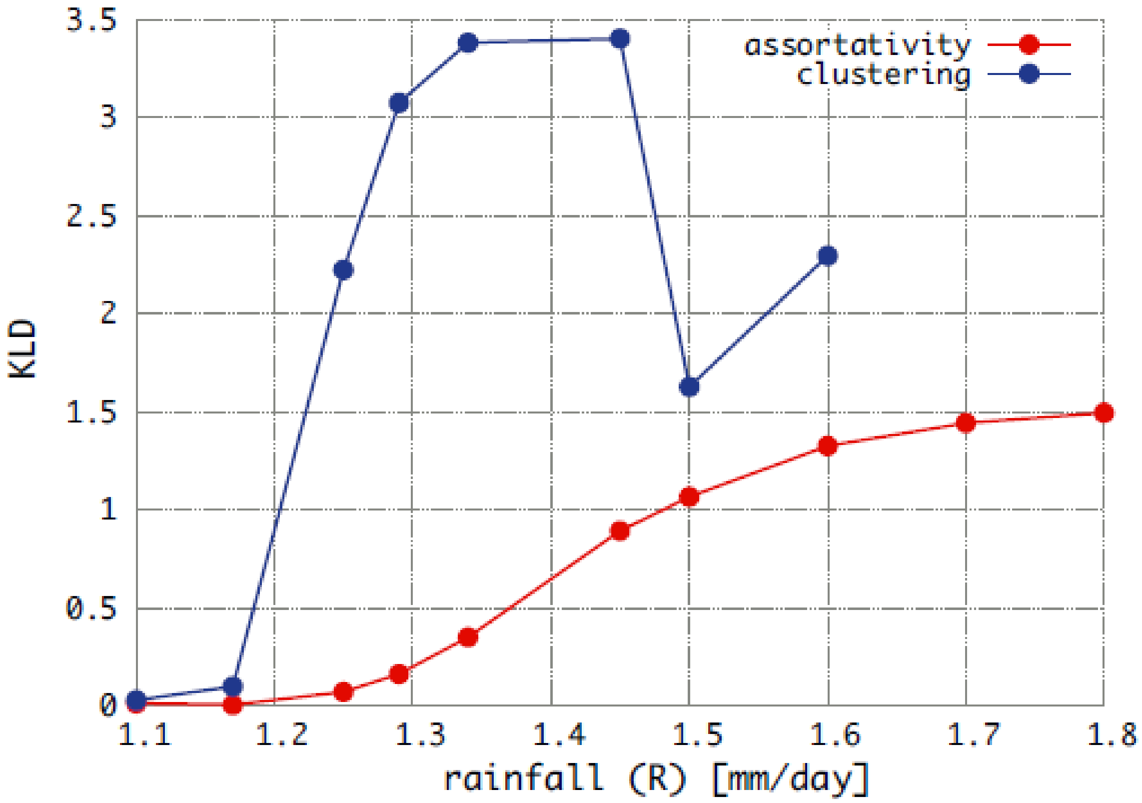
kurtosis

clustering

assortativity



The "Gaussianisation" of the distributions of a_i & c_i values is quantified by the Kullback–Leibler Distance



$$\mathrm{KLD} \equiv \int_{-\infty}^{\infty} \ln\left(\frac{P(x)}{Z(x)}\right) P(x)\, dx.$$

- Open issue: the "Gaussianisation" might be a model-specific feature.
- How to quantify the changes of the network?
- We need a distance to compare graphs.

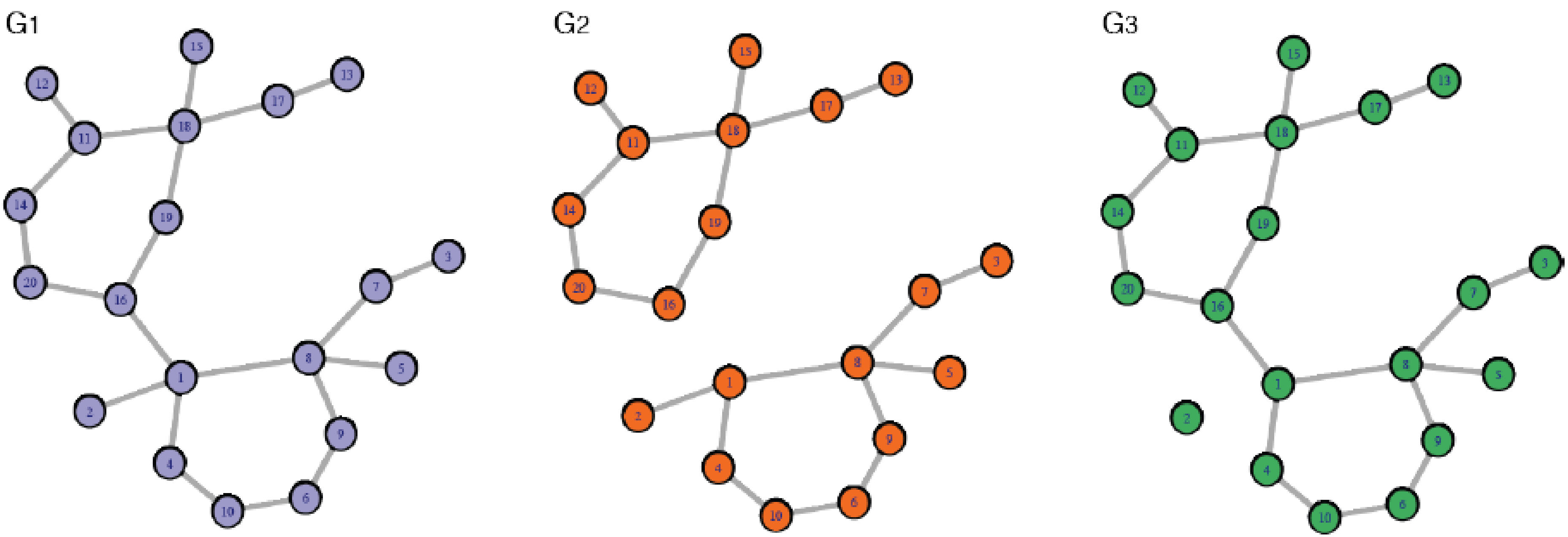
G. Tirabassi et al., Ecological Complexity 19, 148 (2014)

How to compare different networks?

Labelled networks with the same size

- Hamming distance $d_{\text{Hamming}}(y_1, y_2) = \sum_{i \neq j}^{N} \left[A_{ij}^{(1)} \neq A_{ij}^{(2)} \right]$

- Main problem: not all the links have the same importance.



L. Carpi et al, Sci. Reports 9, 4511 (2019)

In order to detect structural differences we need a precise measure to compare networks

- Degree, centrality, assortativity distributions etc. provide *partial* information.
- How to define a measure that contains detailed information about the *global topology* of a network, in a *compact* way?

$\Rightarrow$ Node Distance Distributions (NDDs)

- $p_i(j)$ of node “i“ is the fraction of nodes that are connected to node i at distance j
- If a network has N nodes:

$$\text{NDDs} = \text{vector of N pdfs } \{p_1, p_2, \ldots, p_N\}$$

- If two networks have the same set of NDDs $\Rightarrow$ they have the same diameter, average path length, etc.

How to condense the information contained in the node distance distributions?

- The *Network Node Dispersion (NND*) measures the heterogeneity of the N pdfs $\{p_1, p_2, \ldots, p_N\}$
- Quantifies the heterogeneity of connectivity distances.

$$\mathrm{NND}(G) = \frac{\mathcal{J}(\mathbf{P}_1, \ldots, \mathbf{P}_\mathrm{N})}{\log(d+1)}$$

d = diameter

$$\mathcal{J}(\mathbf{P}_1, \ldots, \mathbf{P}_\mathrm{N}) = \frac{1}{N} \sum_{\mathrm{i,j}} p_\mathrm{i}(j) \log\left(\frac{p_\mathrm{i}(j)}{\mu_\mathrm{j}}\right)$$

$$\mu_\mathrm{j} = \left(\sum_{\mathrm{i}=1}^{N} p_\mathrm{i}(j)\right) / N$$

Dissimilarity between two networks

$$D(G,G') = w_1\sqrt{\frac{\mathcal{J}(\mu_G,\mu_{G'})}{\log 2}} + w_2\left|\sqrt{\mathrm{NND}(G)} - \sqrt{\mathrm{NND}(G')}\right|$$

$w_1 = w_2 = 0.5$

compares the averaged connectivity

compares the heterogeneity of the connectivity distances

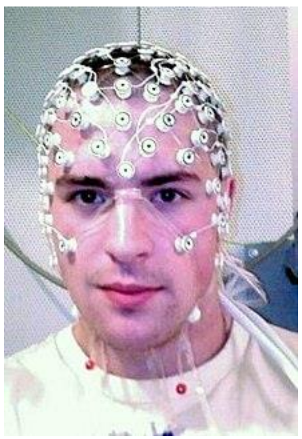
- Extensive numerical experiments demonstrate that isomorphic graphs return ***D=0.***
- Computationally efficient.

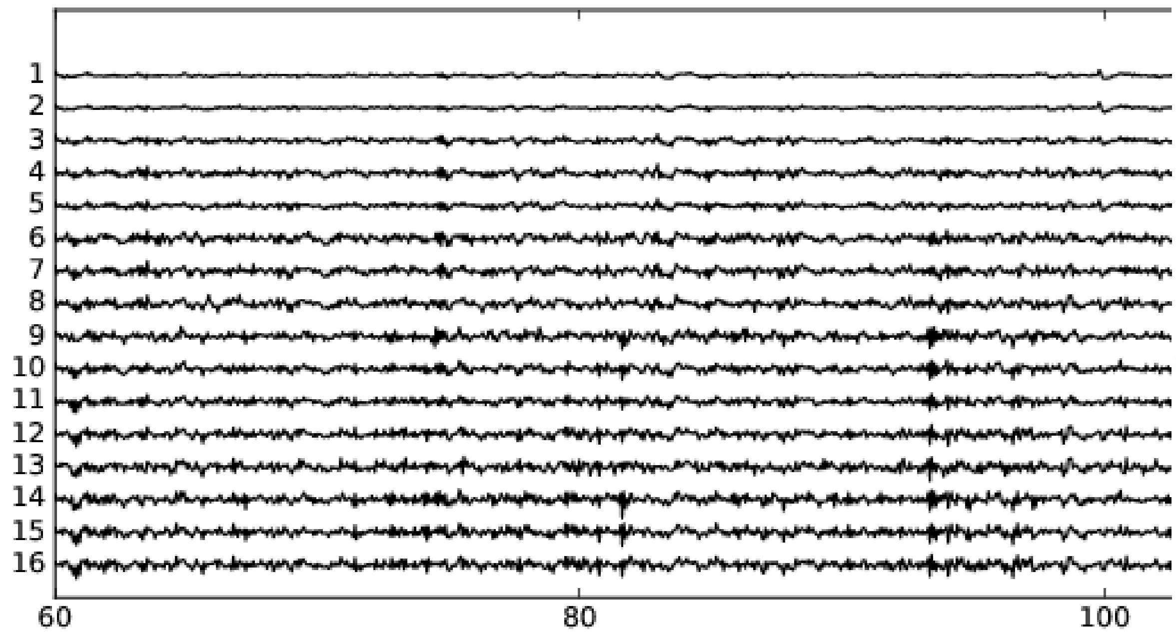
Application: comparing brain networks

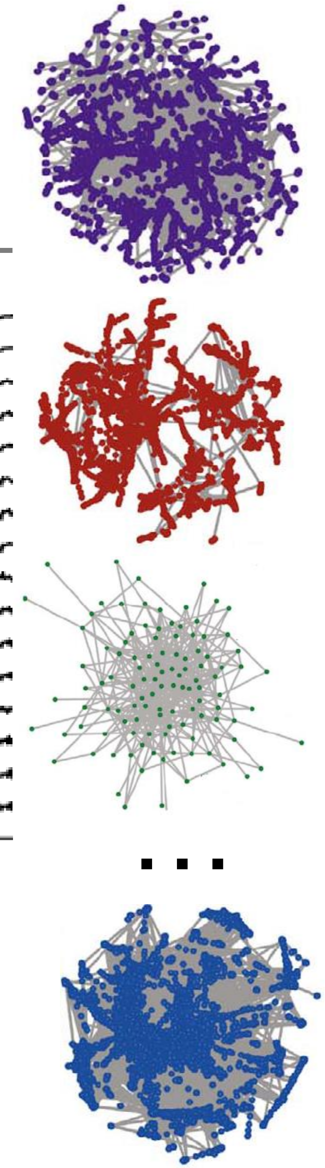
- EEG data
  - https://archive.ics.uci.edu/ml/datasets/eeg+database
  - 64 electrodes placed on the subject’s scalp sampled at 256 Hz during 1s
  - 107 subjects: 39 control and 68 alcoholic
- Use HVG to transform each EEG TS into a network G.
- Weight between two brain regions: **1-*D*(G,G’)**
- The resulting network represents the weighted similarity between the brain regions of an individual.

  $\Rightarrow$ We can compare the different individuals.

For each subject, the time series recorded at each electrode is transformed into a graph



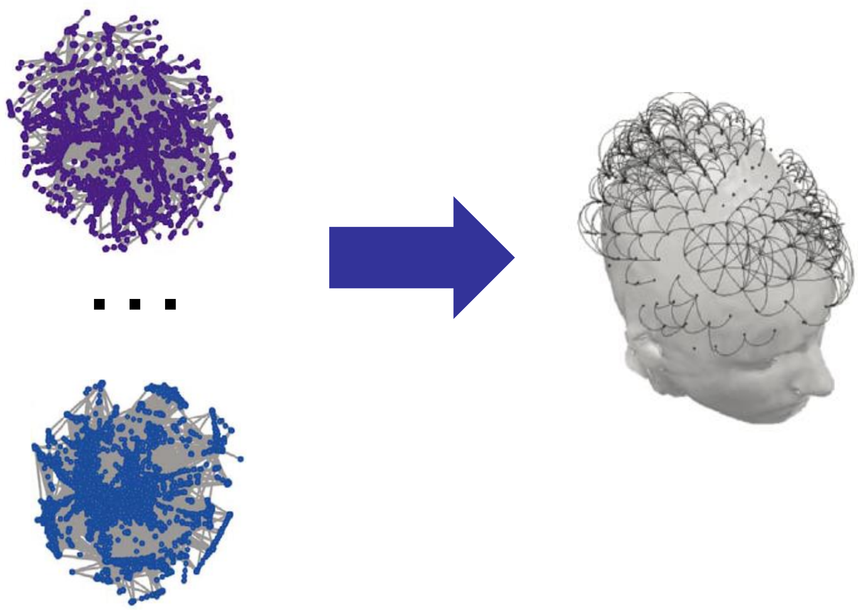




Dataset has 64 channels $\Rightarrow$ 64 networks

The brain network of each subject

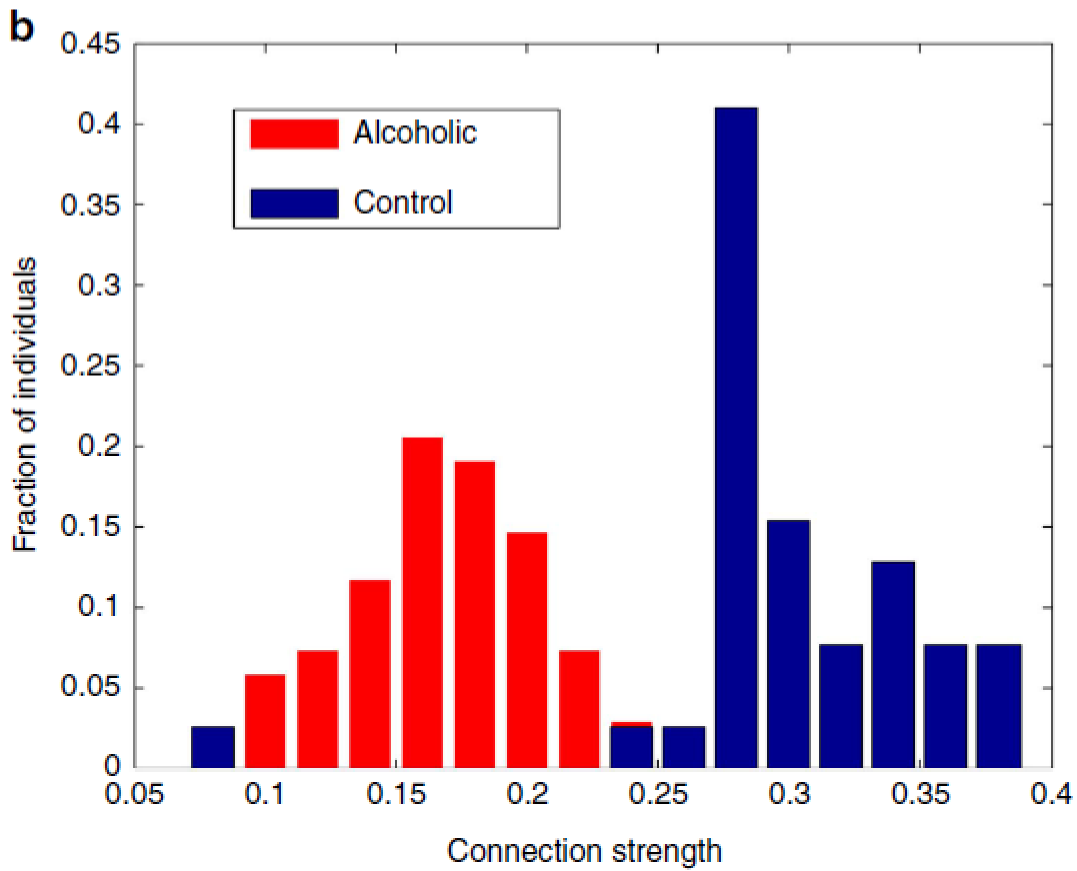
- The weight of the link between two graphs (G, G') representing two brain regions is defined as: **1-*D*(G,G')**



- The resulting network (with 64 nodes=electrodes, all-to-all coupled with weighted links) represents the similarity between the EEG signals in different brain regions of one subject.

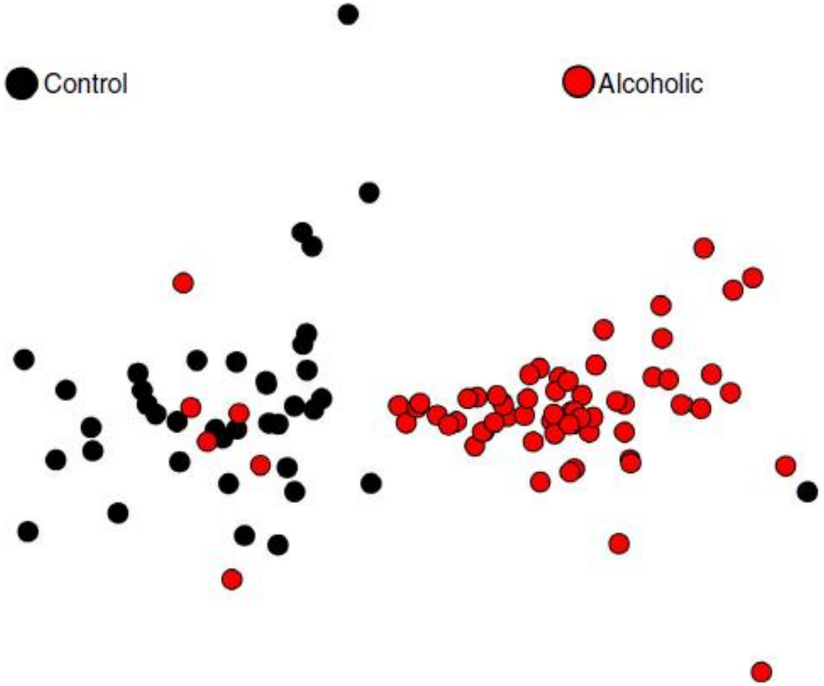
  $\Rightarrow$ We can then compare different subjects.

We identify two brain regions (called ‘nd’ and ‘y’), where the connection strength between these regions is higher in control than in alcoholic subjects.

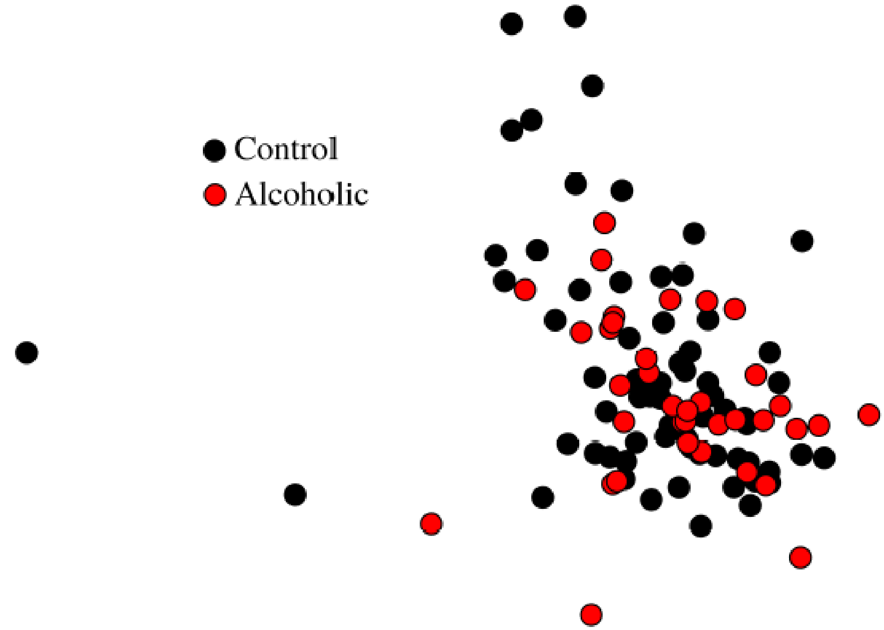


Using the Hamming distance we can not distinguish.

Dissimilarity measure



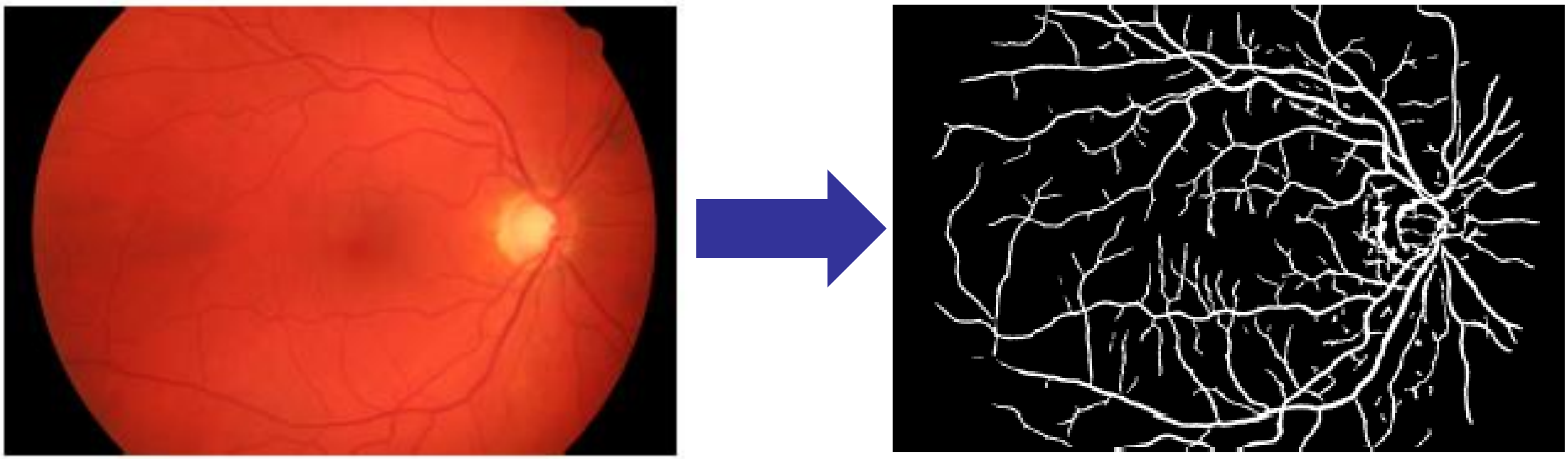
Hamming distance



[T. A. Schieber et al, Nat. Comm. 8, 13928 (2017)]

Retina image classification

Pablo Amil (UPC), **Fabian Reyes** (Mexico) & Irene Sendiña (Madrid)



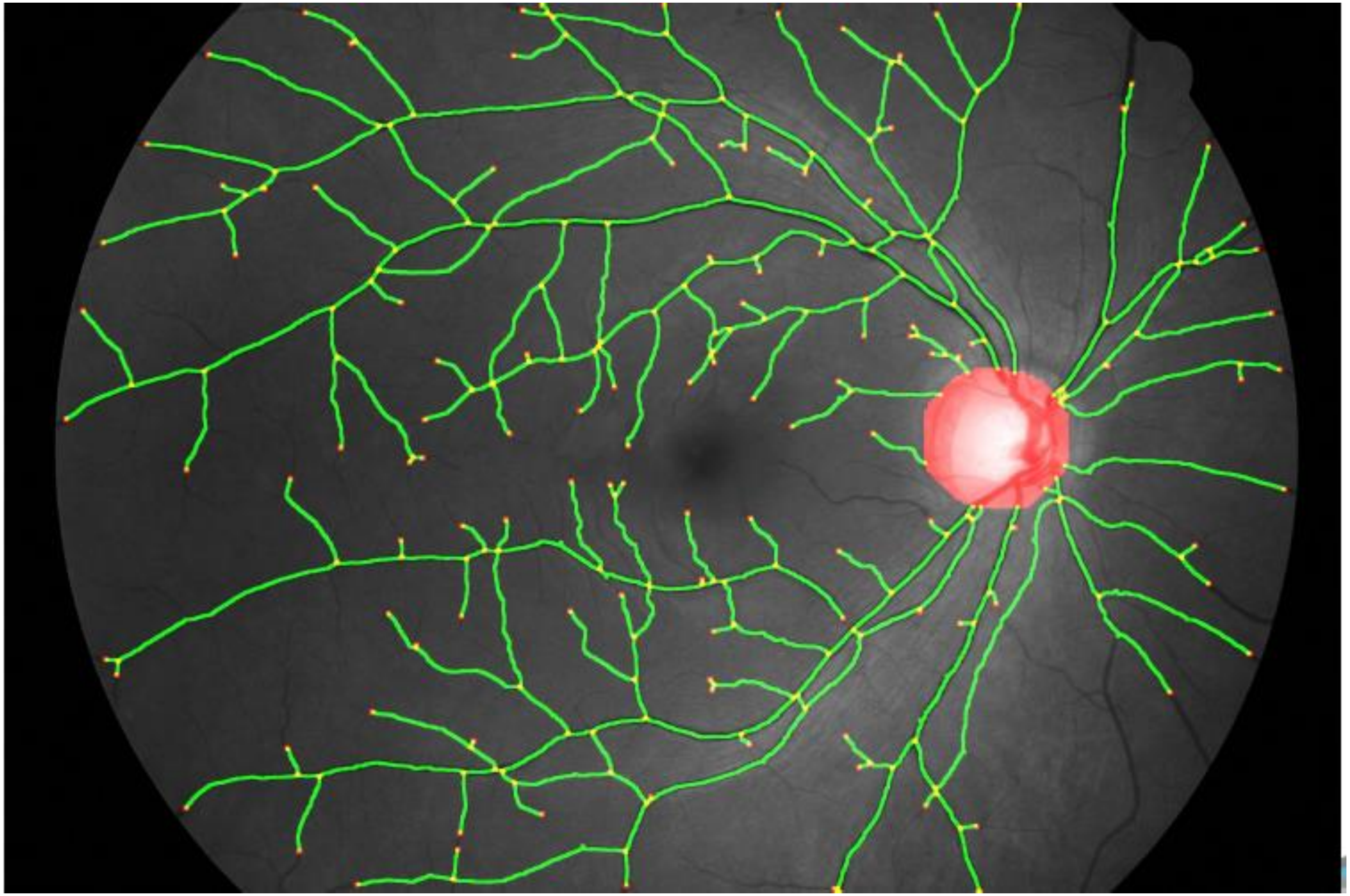
ITN

BE-OPTICAL

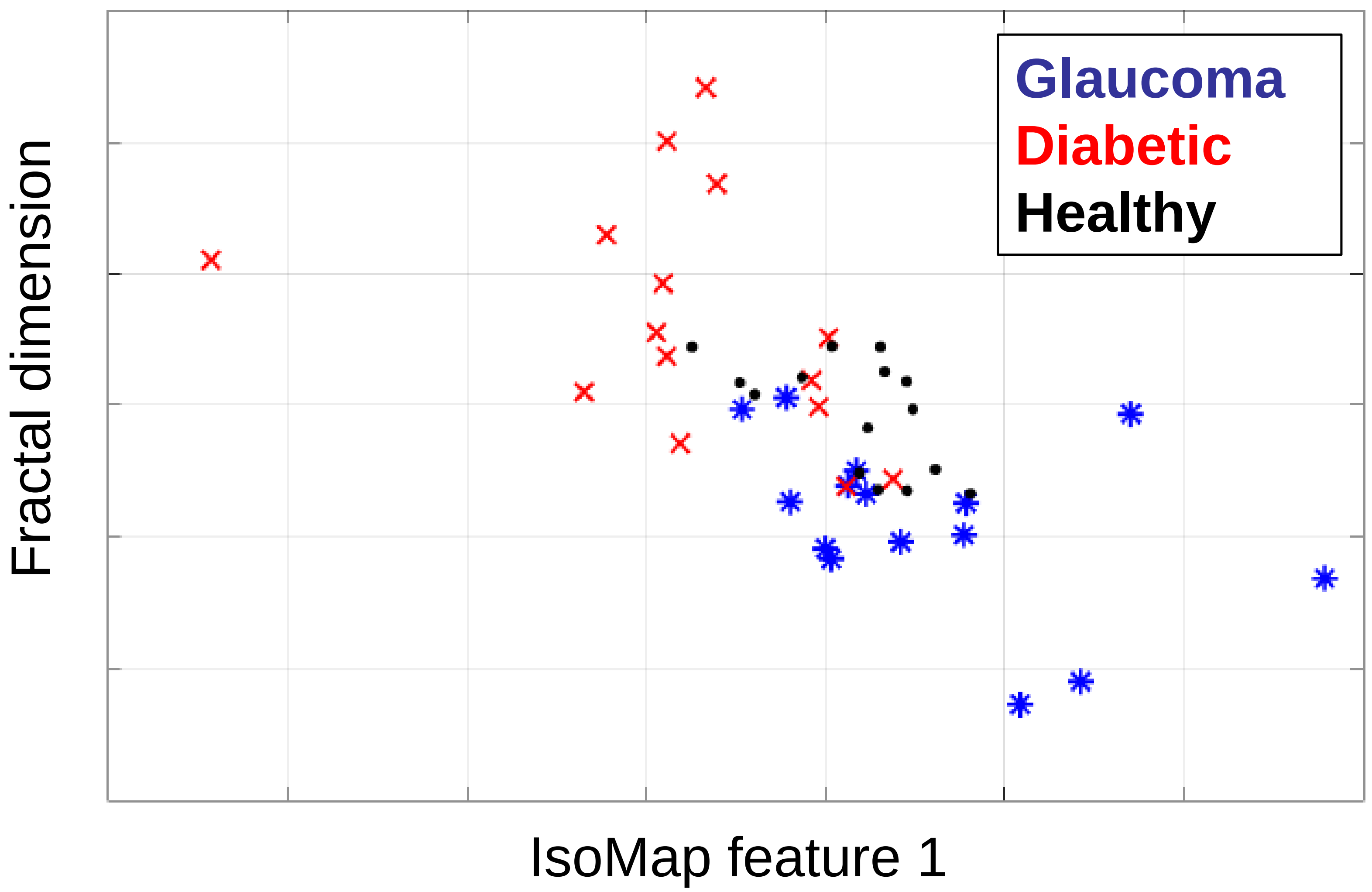
Advanced Biomedical Optical Imaging and Data Analysis

Beoptical.eu

Network identification and analysis of the connectivity paths of the central node



Analysis of the node distance distribution (NDD) of the central node + fractal dimension analysis: promising classification tool



Exercise 3: for the electronic circuits calculate the distance between the functional and the structural networks

Compare the degree distributions of the functional networks constructed in Ex. 2 with the “ground truth”: the degree distribution of the structural network.

Network inference: how to infer the underlying interactions from observed data?

a classification problem

Main problem:

$$S_{ij} > Th \Rightarrow A_{ij} = 1 \text{ else } A_{ij}=0$$

- How to select the threshold?
- In “spatially embedded networks”, nearby nodes have the strongest links.
- How to keep **weak-but-significant** links?

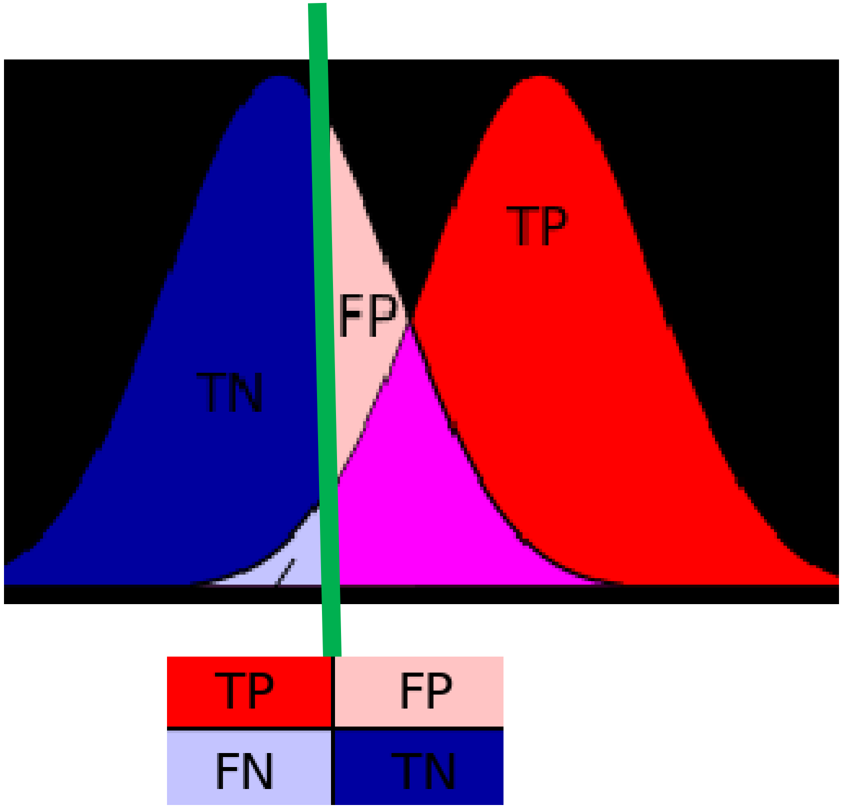
- There are many statistical similarity measures to infer bi-variate mutual interactions from observations, i.e., to classify:
  - the interaction exists (is significant)
  - the interaction does not exists (or is not significant)

	Predicted: NO	Predicted: YES
Actual: NO	TN	FP
Actual: YES	FN	TP

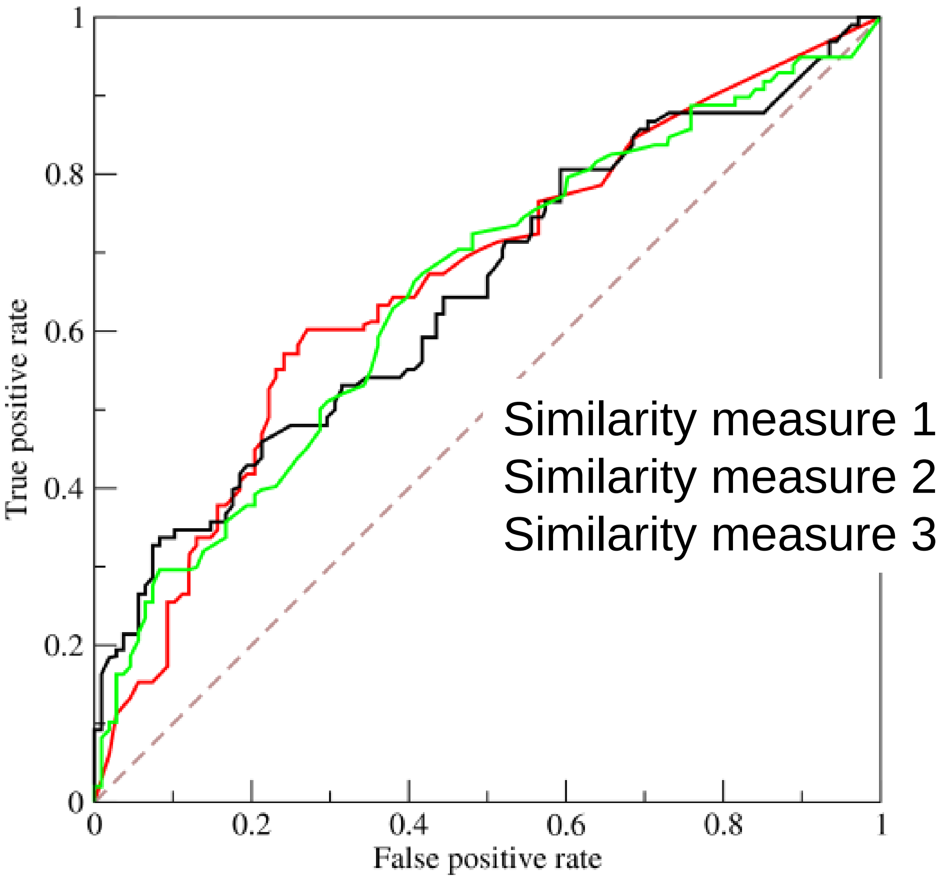
Confusion matrix

- ***Accuracy***: How often is the classifier correct? **(TP+TN)/total**
- ***Misclassification*** (Error Rate): How often is it wrong? **(FP+FN)/total**
- ***True Positive Rate*** (TPR, Sensitivity): When it's yes, how often does it predict yes? **TP/actual yes**
- ***False Positive Rate*** (FPR) : When it's no, how often does it predict yes? **FP/actual no**
- ***Specificity*** (1 – FPR) : When it's no, how often it predicts no? **TN/actual no**
- ***Precision*** (Positive Predictive Value): When it predicts yes, how often is it correct? **TP/predicted yes**
- ***Negative Predictive Value***: When it predicts no, how often is it correct? **TN/predicted no**
- ***Prevalence***: How often does the yes condition actually occur in the sample? **actual yes/total**

Receiver operating characteristic (ROC curve)



Source: wikipedia



Our goal

- To compare the performance of different statistical similarity measures for inferring interactions from observations.

- Using a “toy model” where **we know** the underlying equations and interactions and so we can check the performance of the different measures in inferring the interactions.

Kuramoto oscillators in a random network

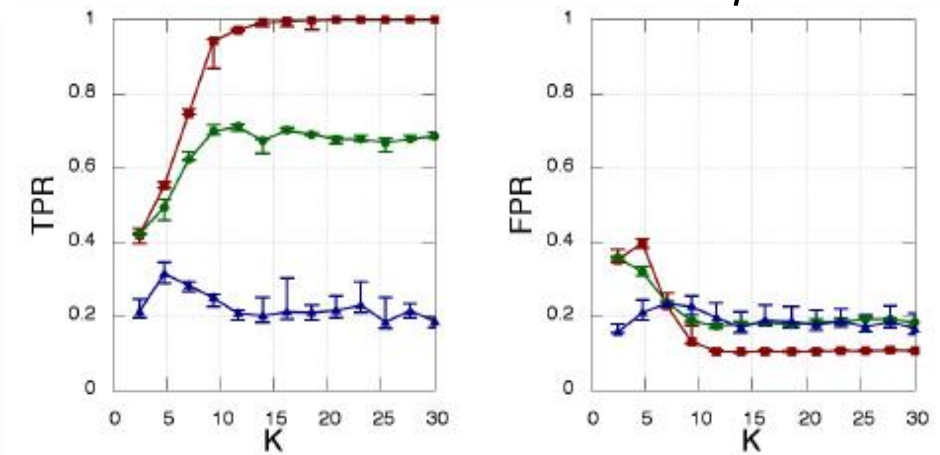
$$d\theta_i = \omega_i dt + \frac{K}{N}\sum_{j=1}^{N} A_{ij}\sin(\theta_j - \theta_i)dt + D\, dW_t^i$$

A_{ij} is a symmetric random matrix;
N=12 time-series, each with 10^4 data points.

CC MI MIOP

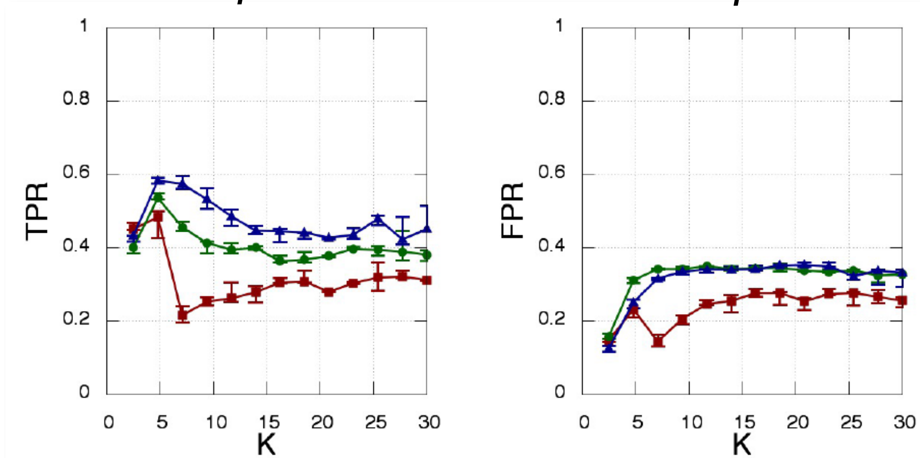
Phases (θ)

True positives *False positives*



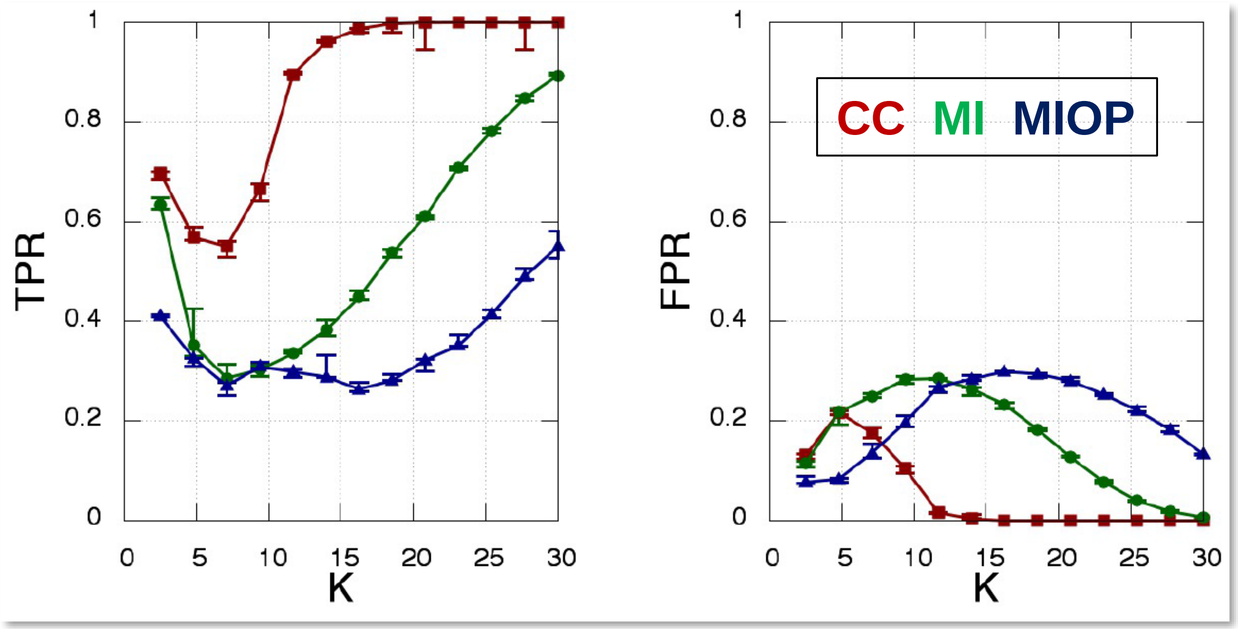
"Observable" Y=sin(θ)

True positives *False positives*



Results of a 100 simulations with different oscillators' frequencies, random matrices, noise realizations and initial conditions.
For each K, the threshold was varied to obtain optimal reconstruction.

Instantaneous frequencies (dθ/dt)



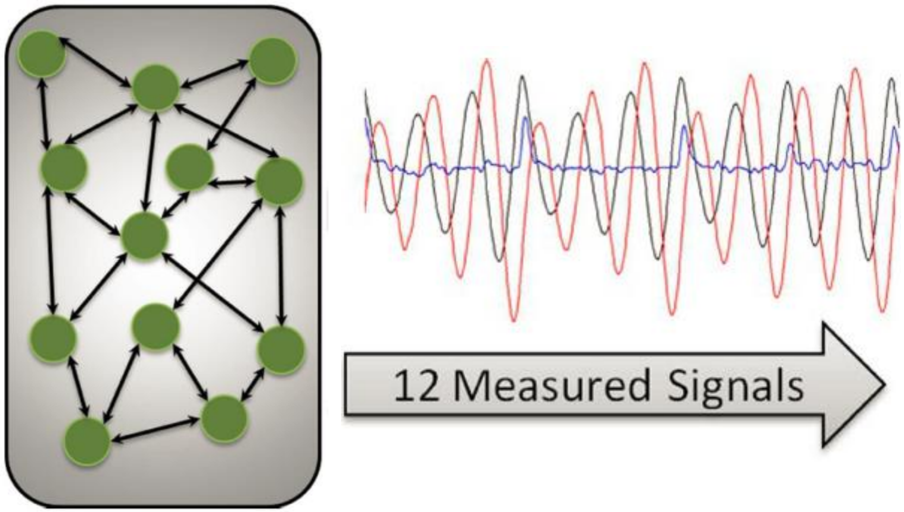
Perfect network inference is possible!

BUT

- the number of oscillators is small (12),
- the coupling is symmetric ($\Rightarrow$ only 66 possible links) and
- the data sets are long (10^4 points)

[G. Tirabassi et al, Sci. Rep. **5** 10829 (2015)]()

We also analyzed experimental data recorded from 12 chaotic Rössler electronic oscillators (symmetric and random coupling)



The Hilbert Transform was used to obtain phases from experimental data

G. Tirabassi et al, Sci. Rep. **5** 10829 (2015)

- Kuramoto Oscillators' Network

$$\theta_i$$

$$f_i = \dot{\theta}_i$$

$$Y_i = \sin(\theta_i)$$

- Rössler Oscillators' Network

$$\varphi_i = HT(x_i)$$

$$f_i = \dot{\varphi}_i$$

$$x_i$$

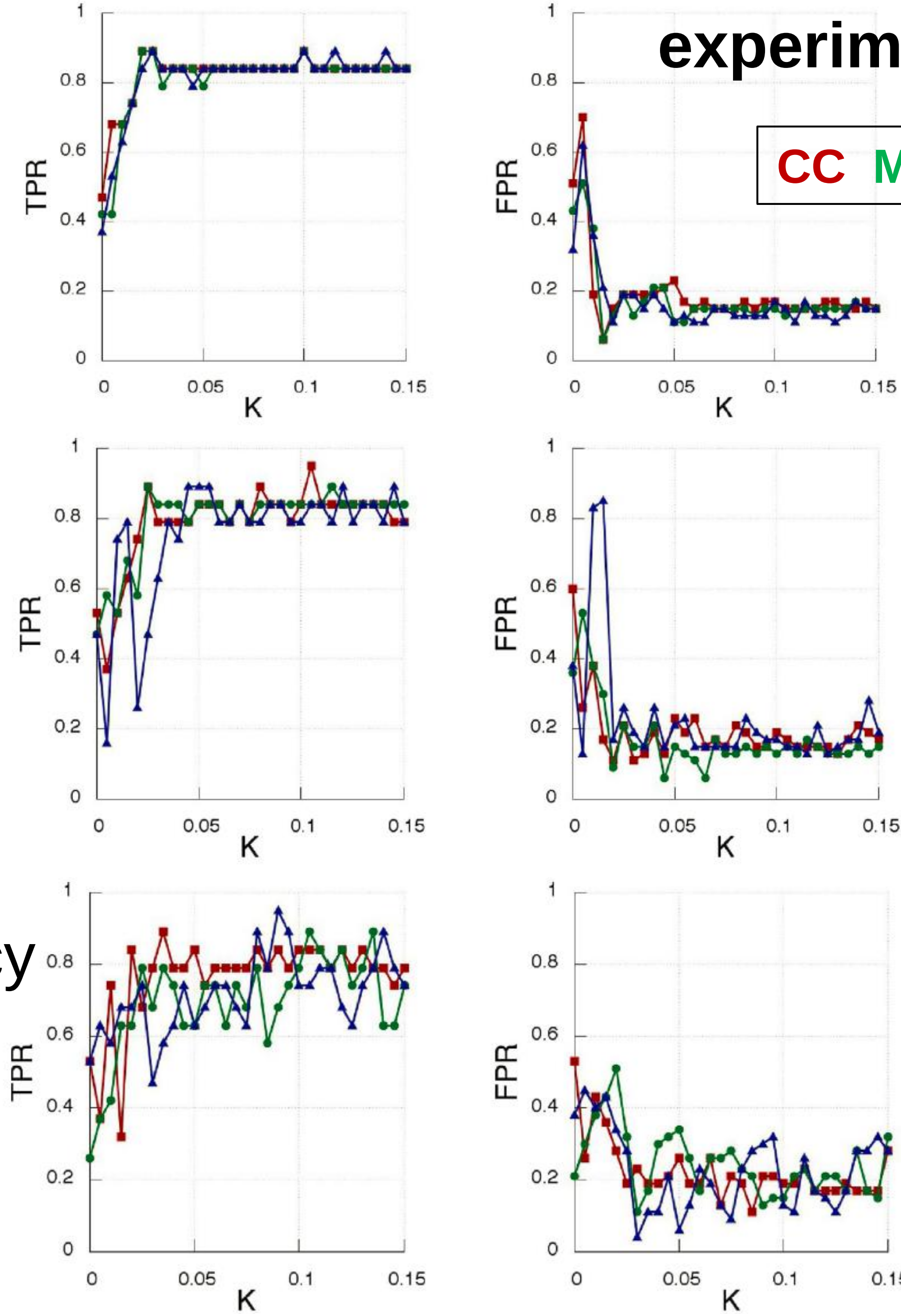
Results obtained with experimental data

CC MI MIOP

Observed variable (x)

Hilbert phase

Hilbert frequency

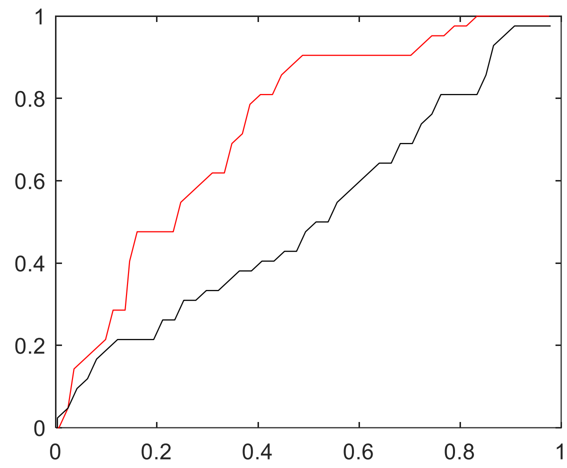


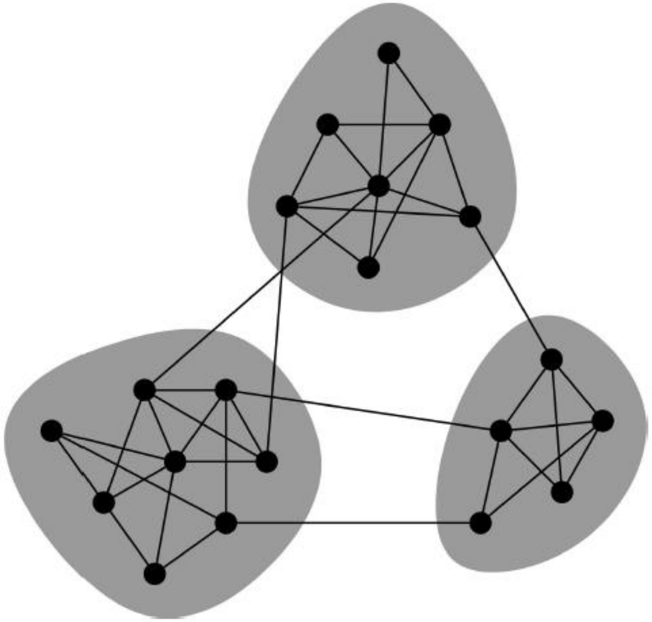
– No perfect reconstruction

– No important difference among the 3 methods & 3 variables

Exercise 4: for the 28 electronic circuits, can we infer the structural network?

Calculate the ROC curve for different coupling strengths.



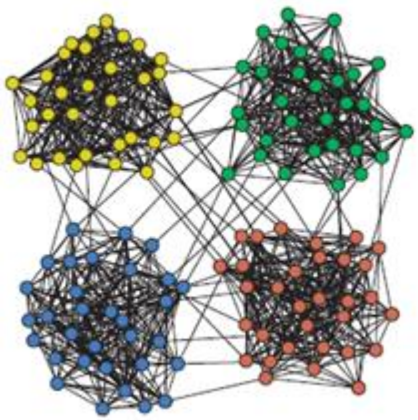


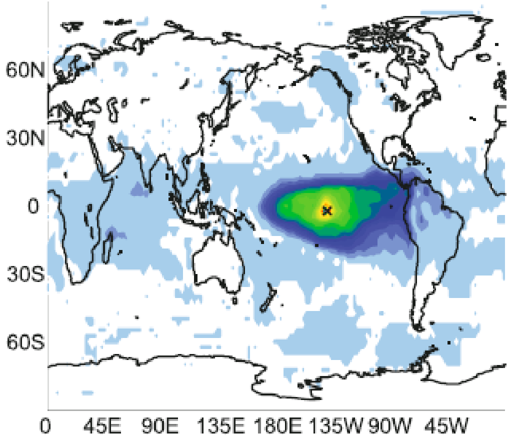
Community detection

Climate "communities"

How to identify regions with similar climate?

- Goal: to construct a network in which regions with similar climate (e.g., continental) are in the same "community".
- Problem: not possible with the "usual" correlation-based method to construct the network because NH and SH are only indirectly connected.





Network construction based on similar symbolic dynamics

- Step 1: transform SAT anomalies in each node in a sequence of symbols (we use ordinal patterns)

  s_i = {012, 102, 210, 012…} s_j = {201, 210, 210, 012, …}

- Step 2: in each node compute the transition probabilities

  $TP^{i}_{\alpha\beta} = \#(\alpha \rightarrow \beta)/N$

- Step 3: define the weights $$w_{ij} = \frac{1}{\sum_{\alpha\beta}\left(TP^{i}_{\alpha\beta} - TP^{j}_{\alpha\beta}\right)^2}$$

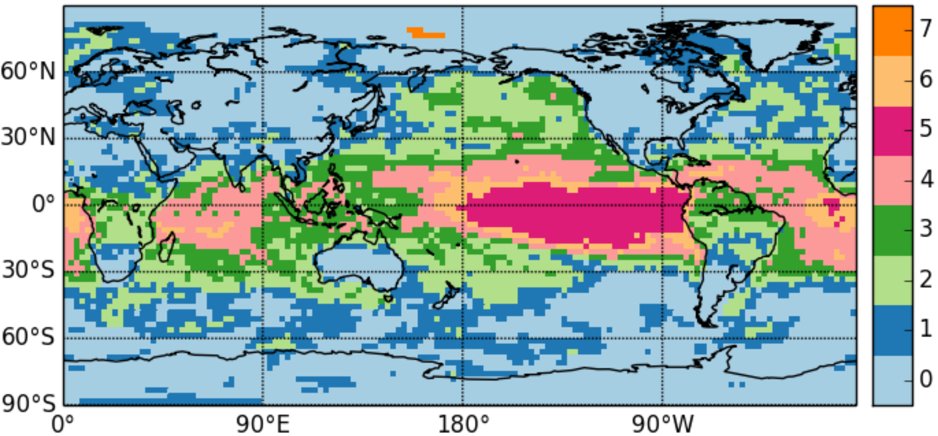
  High weight if similar symbolic "language"

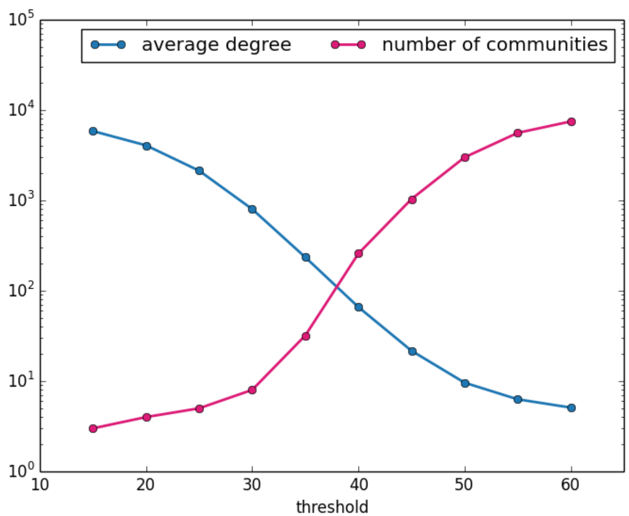
- Step 4: threshold w_{ij} to obtain the adjacency matrix.

- Step 5: run a *community detection algorithm* (*Infomap*).

Results

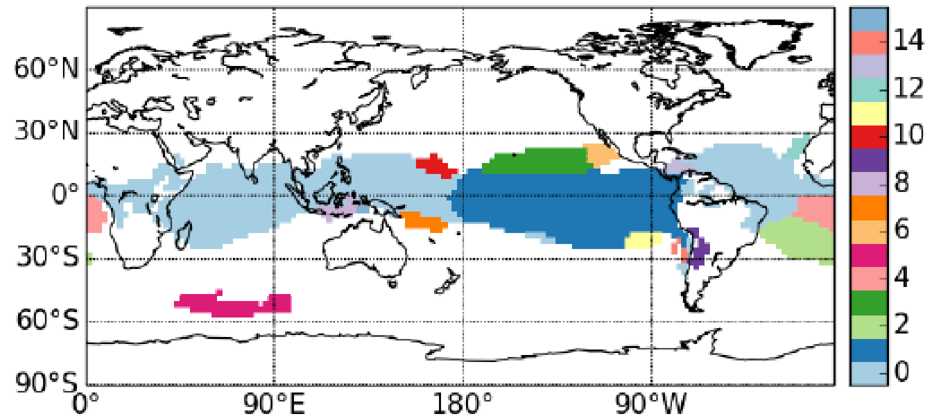
TP Network

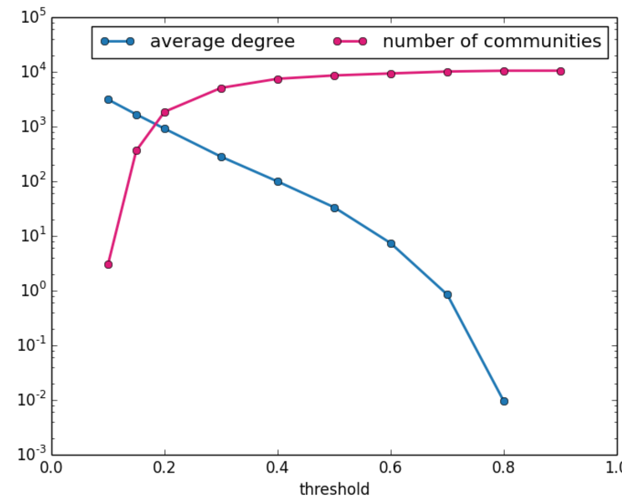




CC Network

(only the largest 16)





G. Tirabassi and C. Masoller, "*Unravelling the community structure of the climate system by using lags and symbolic time-series analysis*", Sci. Rep. **6**, 29804 (2016).

Community detection algorithms

- *Infomap* (http://www.mapequation.org/code.html) and many others.

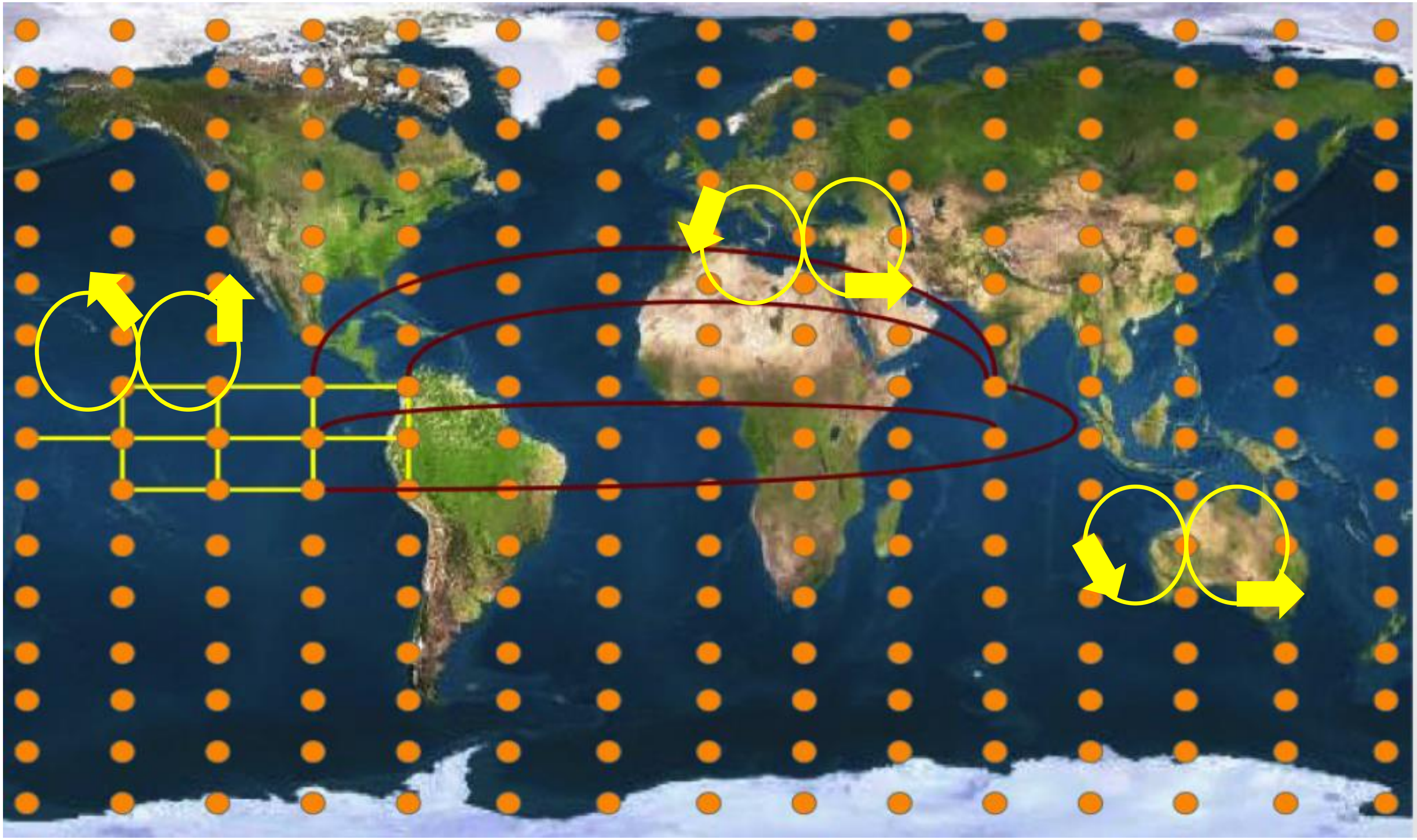
- *Infomap* clusters tightly interconnected nodes into modules and detects nested modules.

- Many other algorithms have been proposed.

- Further reading: S. Fortunato, “*Community detection in graphs*”, Phys. Rep. 486, 75 (2010).

How to detect phase synchronization in climate data?

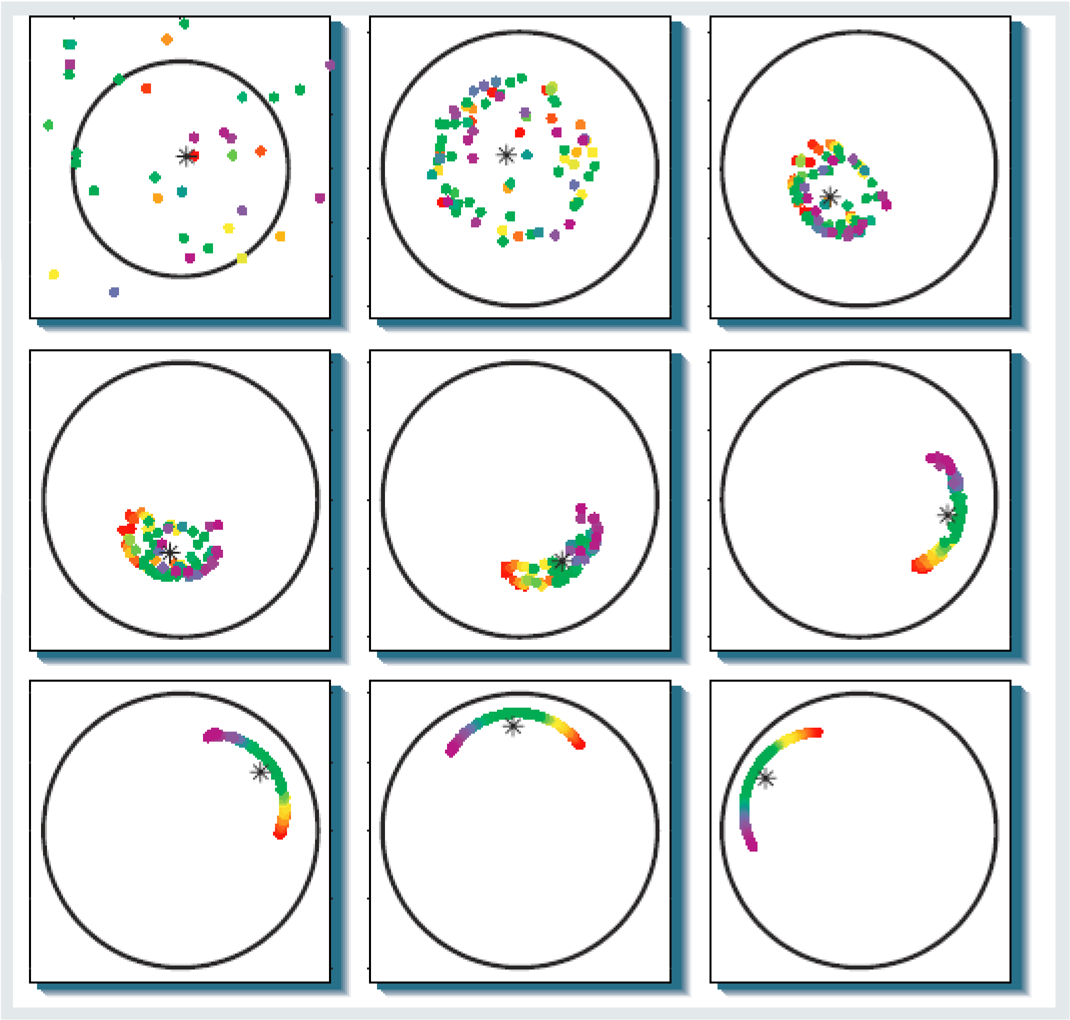
Network of individual oscillators



Quantifying phase synchronization

- Kuramoto order parameter

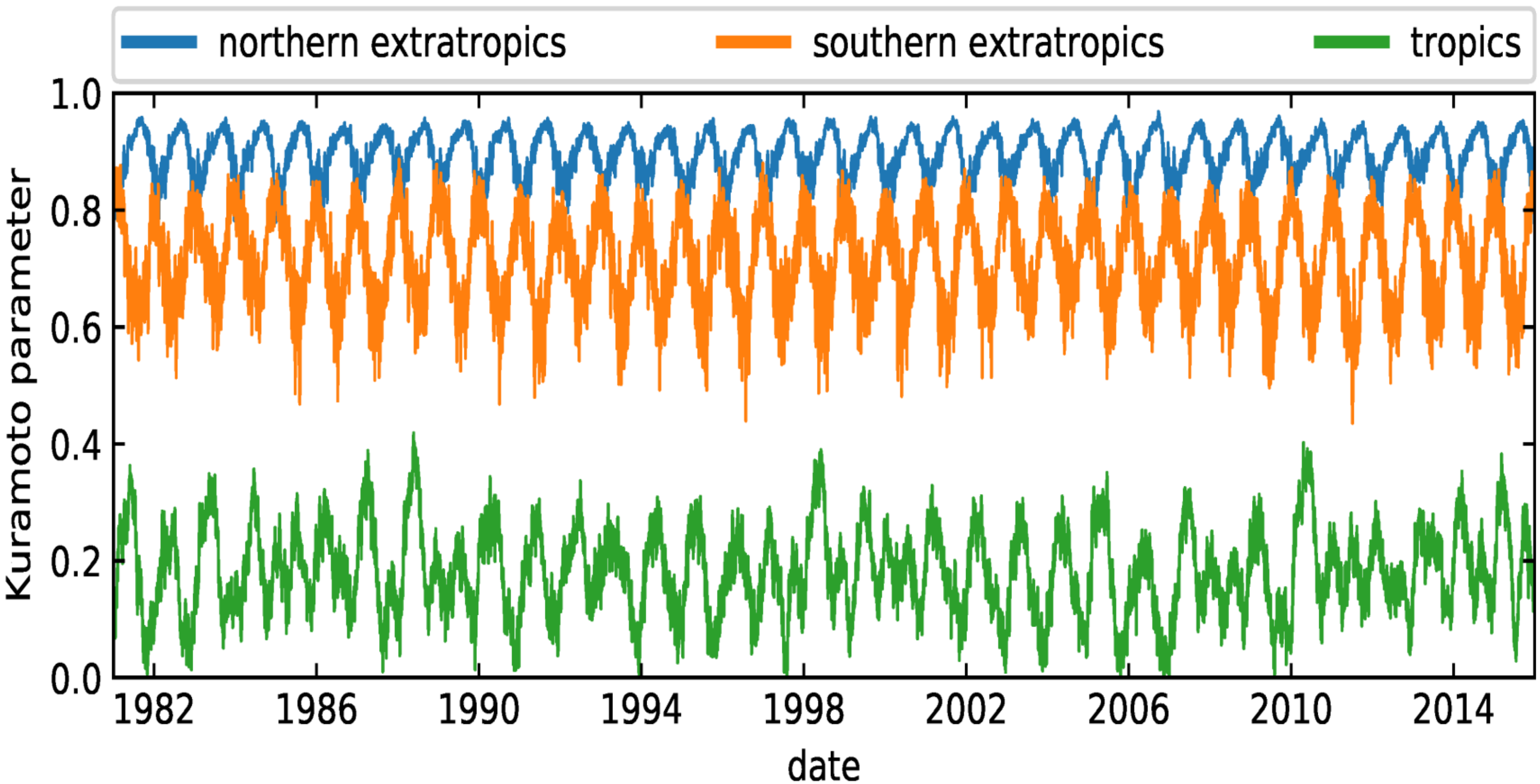
$$r(t) = \left| \frac{1}{N} \sum_{j=1}^{N} e^{i\theta_j(t)} \right|$$



Steven H. Strogatz, Nature 2001

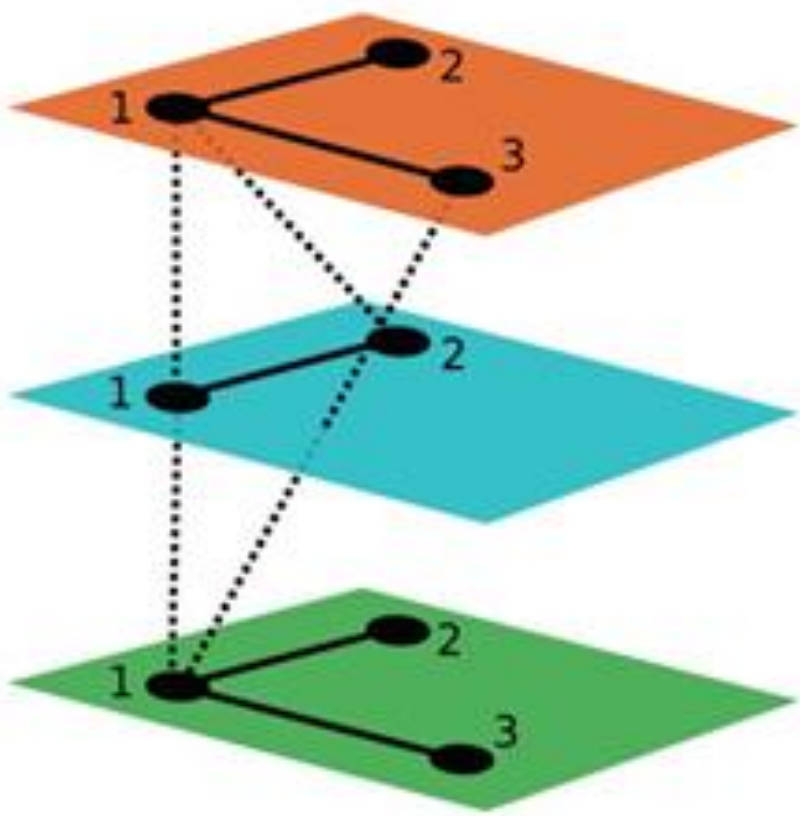
Hilbert transform ⇒ phase time series ⇒area-weighted Kuramoto order parameter

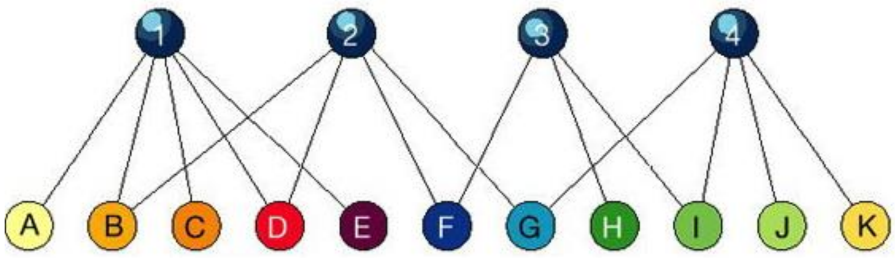
$$r(t) = \left| r(t) e^{i\psi(t)} \right| = \left| \frac{\sum_{j \in S} w_j e^{i\varphi_j(t)}}{\sum_{j \in S} w_j} \right|$$

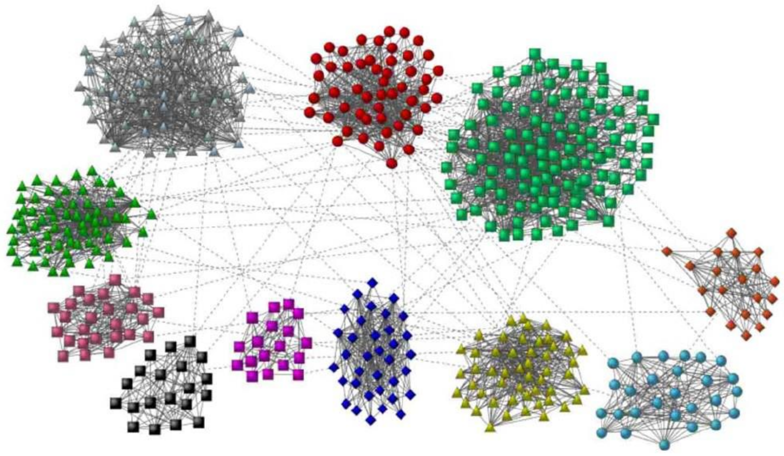


Generalizations of complex network analysis

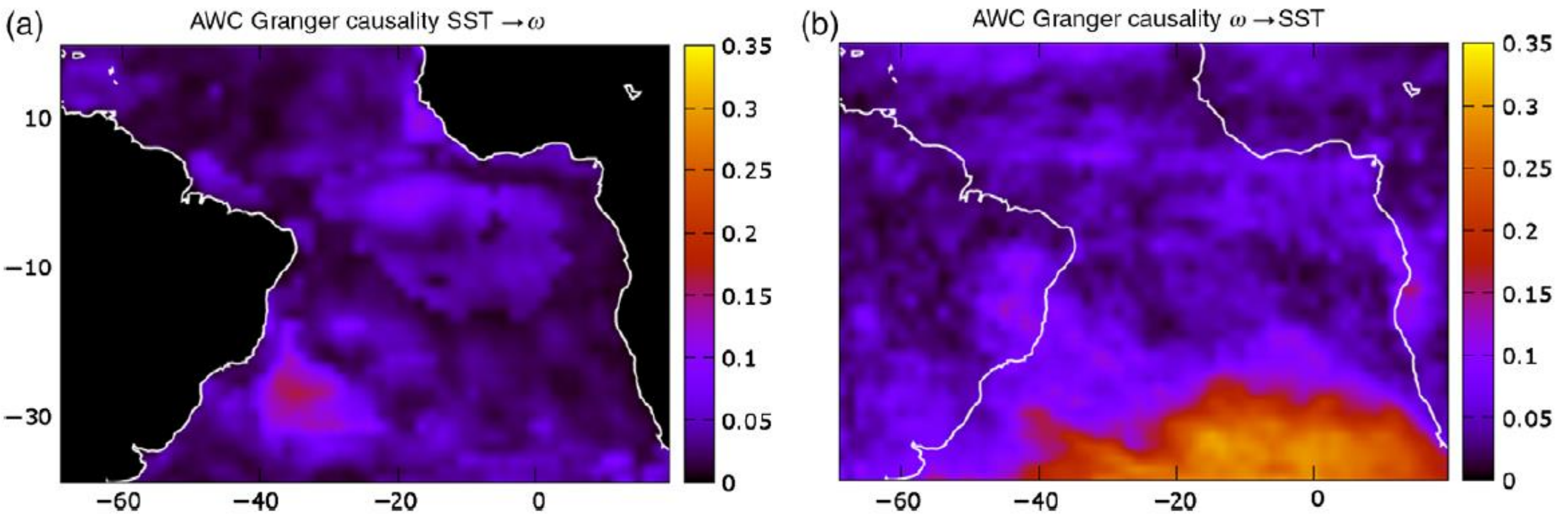
Network structures: Multilayer, multiplex, bipartite, networks of networks and many others







Example of a bilayer climate network representing ocean-precipitation interactions



Color code shows the area-weighted connectivity (weighted degree) of a bilayer network where the links are defined using Granger causality (only GCE values at 99% confidence level have been considered).

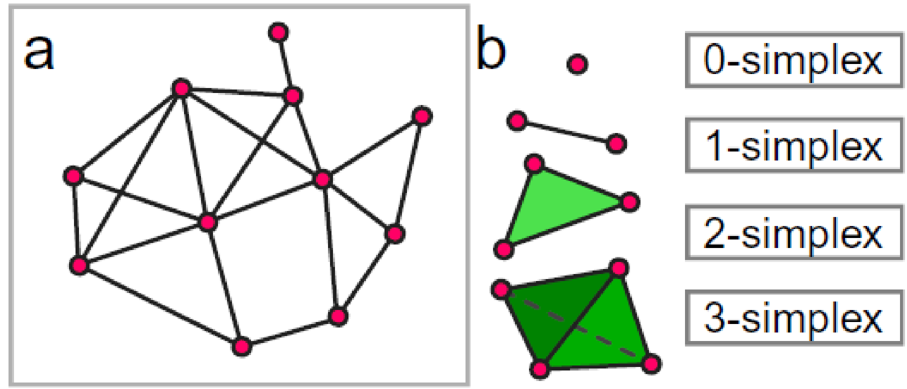
SST = Surface sea temperature

ω = vertical wind velocity at 500 hPa (precipitation proxy)

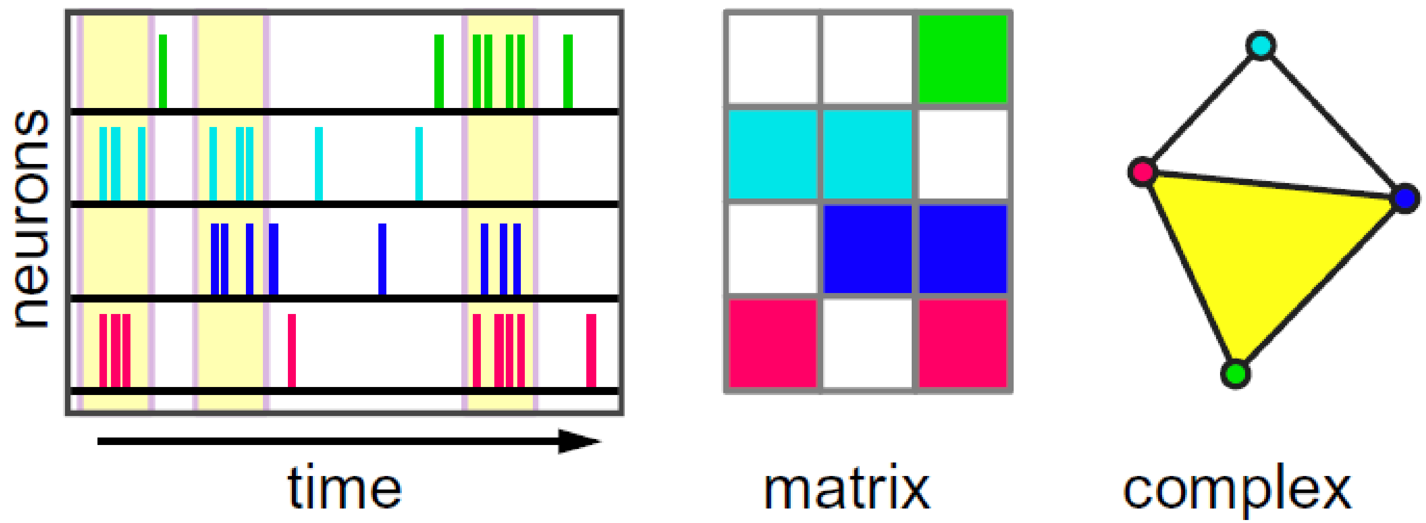
Tirabassi, Masoller and Barreiro, Int. J. of Climatology, 35, 3440 (2015)

A basic limitation of network analysis

- Links represent interactions between pairs of nodes.
- ***Simplicial complexes*** represent interactions among several nodes.



Example



Giusti et al., J Comput Neurosci (2016) 41:1–14

Concluding

Take home messages

- There are many methods for inferring the underlying connectivity of a complex system from the observed output signals.
- Different methods infer different networks.
- Comparing (quantifying differences) between networks is challenging.
- Different sets of “communities” (clusters) can be uncovered depending on the property that is analyzed.

References

- M. Barreiro, et. al, Chaos 21, 013101 (2011)
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- T. A. Schieber et al, Nat. Comm. 8, 13928 (2017)

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http://www.fisica.edu.uy/~cris/