

VI Jornadas ALAMA: Laplacian and M-matrices on Graphs
2023 Barcelona, May 11-12

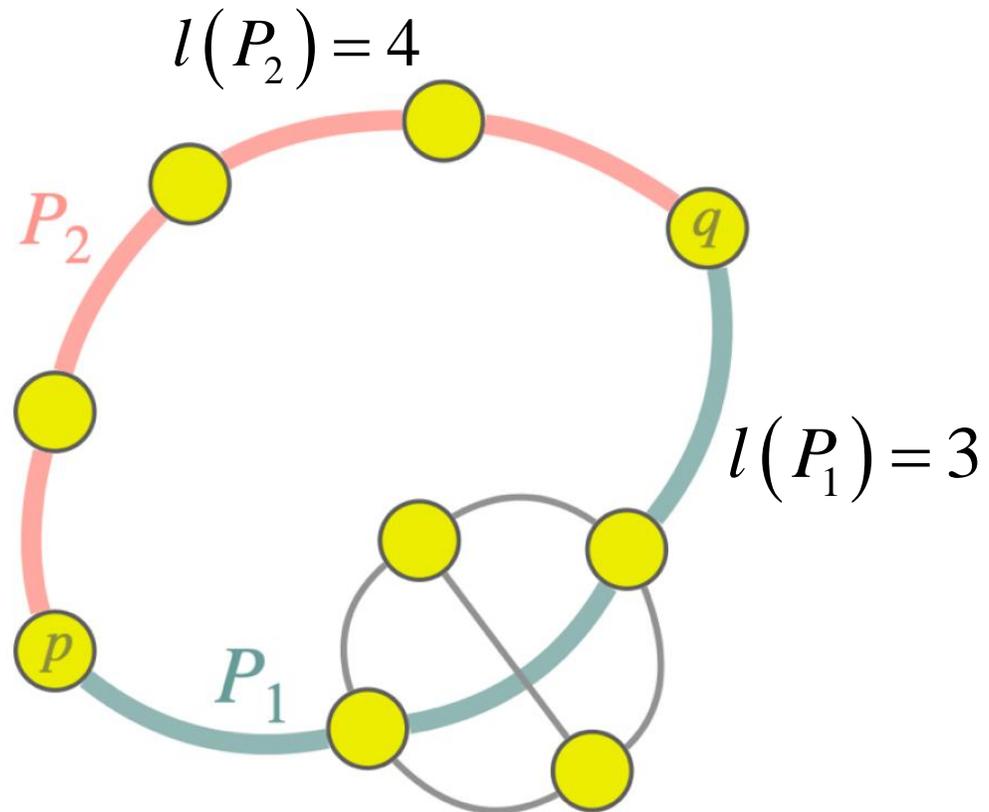
Spherical Euclidean matrices and effective resistance in graphs

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Motivation

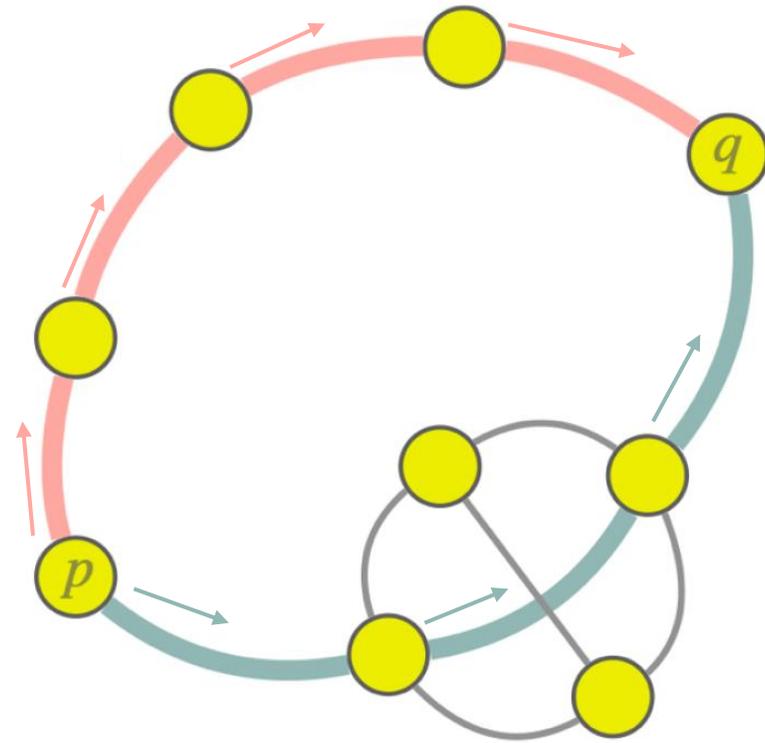


Hitting time: the time (number of steps) that a random walker, departing from p , takes to hit by the first time the node q .

Excess time: the time (number of steps) taken by a random walker, departing from p , to arrive to q in comparison with a ballistic walk.

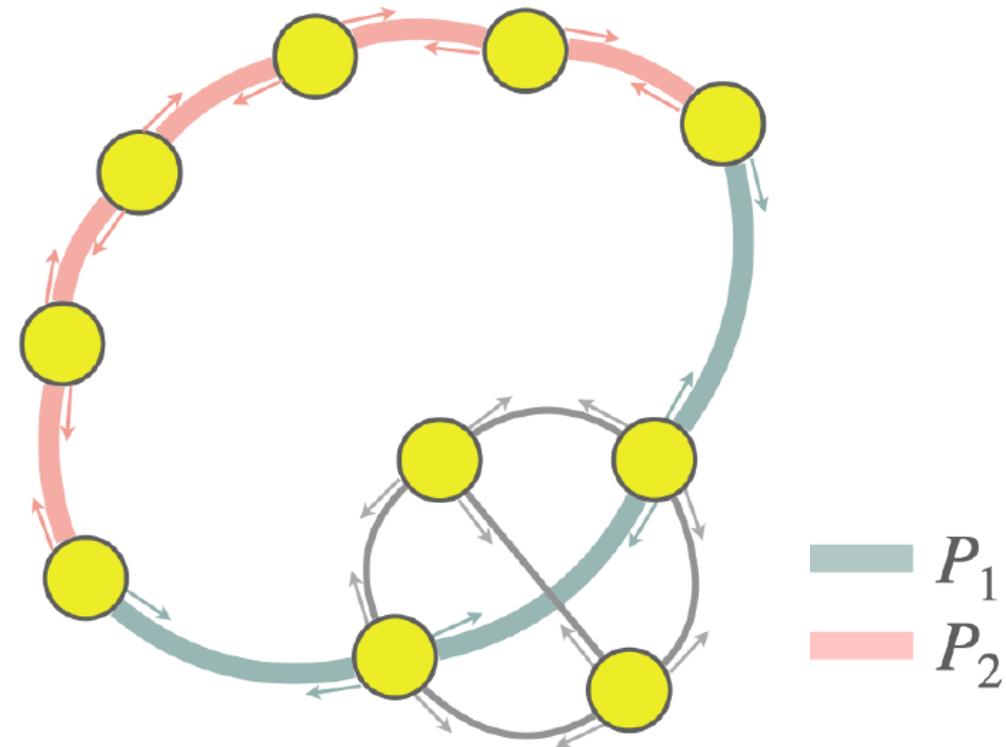
	P₁	P₂
Hitting time	10.9	6.9
Excess time	2.7	1.38

“a *routing/navigation process* implies that communication flows from a specific source to a specific target along the fastest or most direct route, which implies *global knowledge about the network topology*.”



VS.

“a *diffusion process* implies that communication occurs in the absence of specific targets, or that, even if targets are specified, *a lack of knowledge about global network topology prevents particles or messages from taking shortest paths*.”



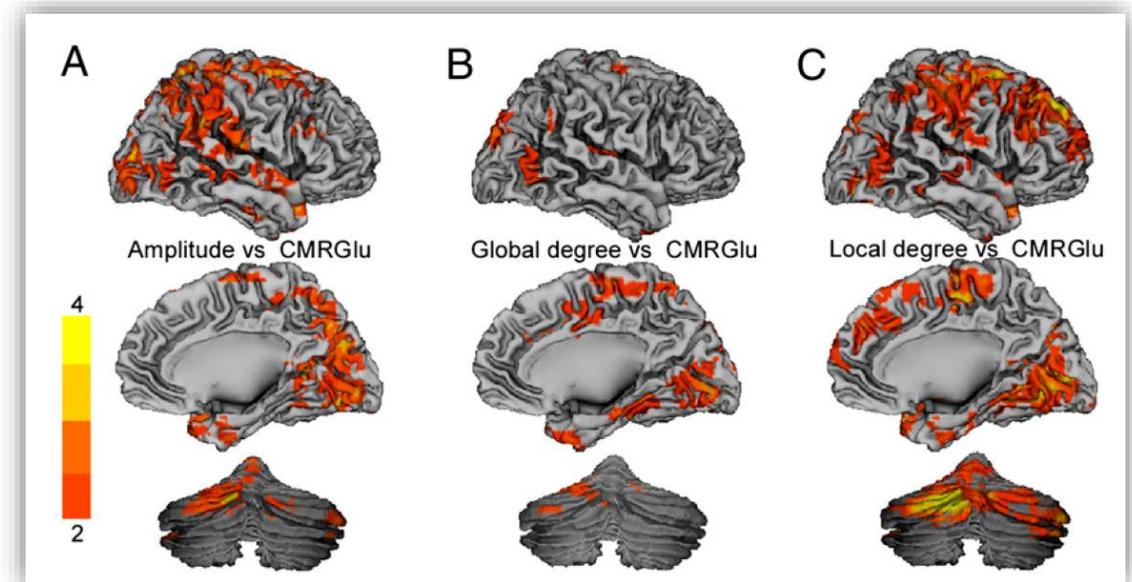
Affirmations like:

*“The shortest path plays an important role in the **information transmission of a brain network**, and it is a very important measure to describe the internal structure of the brain network. The **shortest path can transmit the information more quickly and reduce brain consumption**.”*

Liu et al.: *Complexity* (2017), 8362741.

Contrasts with facts like:

*“A higher degree of connectivity was associated with **nonlinear increases in metabolism**.”*



Tomasi et al.: *Proc. Nat. Acad. Sci. USA* **110** (2013) 13642–13647.

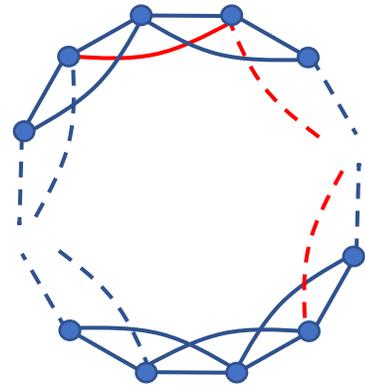
The idea of “shortest path” is implicit in the Watts-Strogatz and Barabási-Albert models

Collective dynamics of ‘small-world’ networks

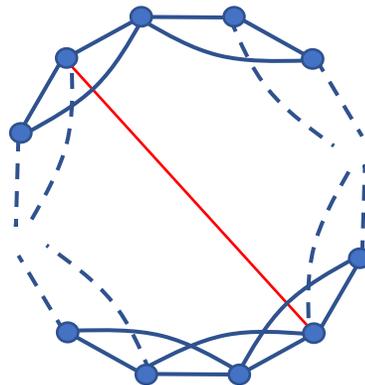
Nature 393 (1998) 440-442



Watts



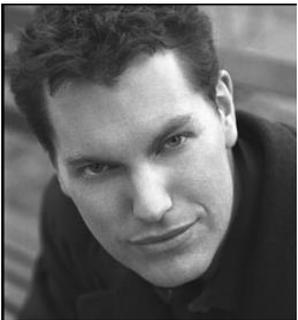
Strogatz



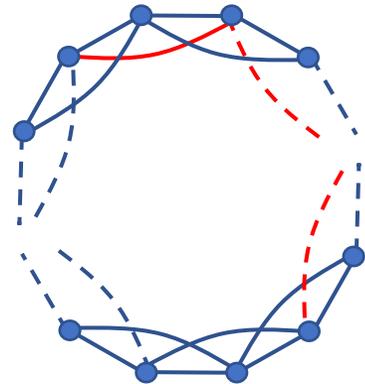
Network models

The idea of “shortest path” is implicit in the Watts-Strogatz and Barabási-Albert models

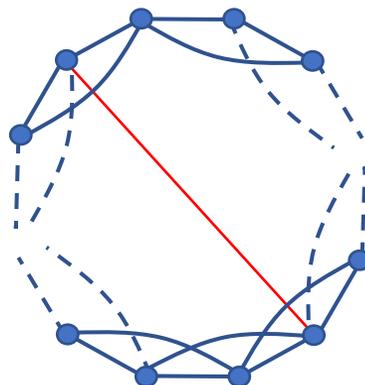
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Watts



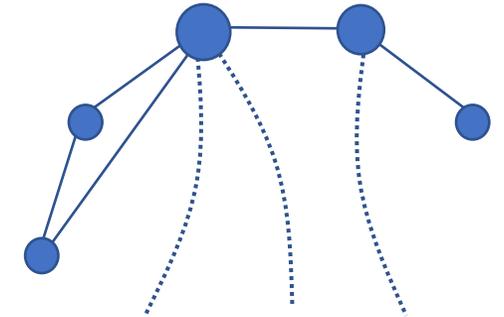
Strogatz



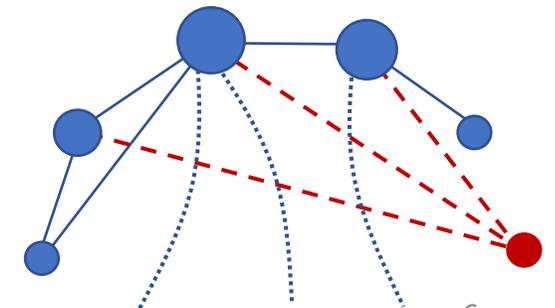
Emergence of Scaling in Random Networks
Science 286 (1999) 509-512



Barabási

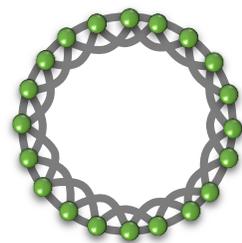


Albert

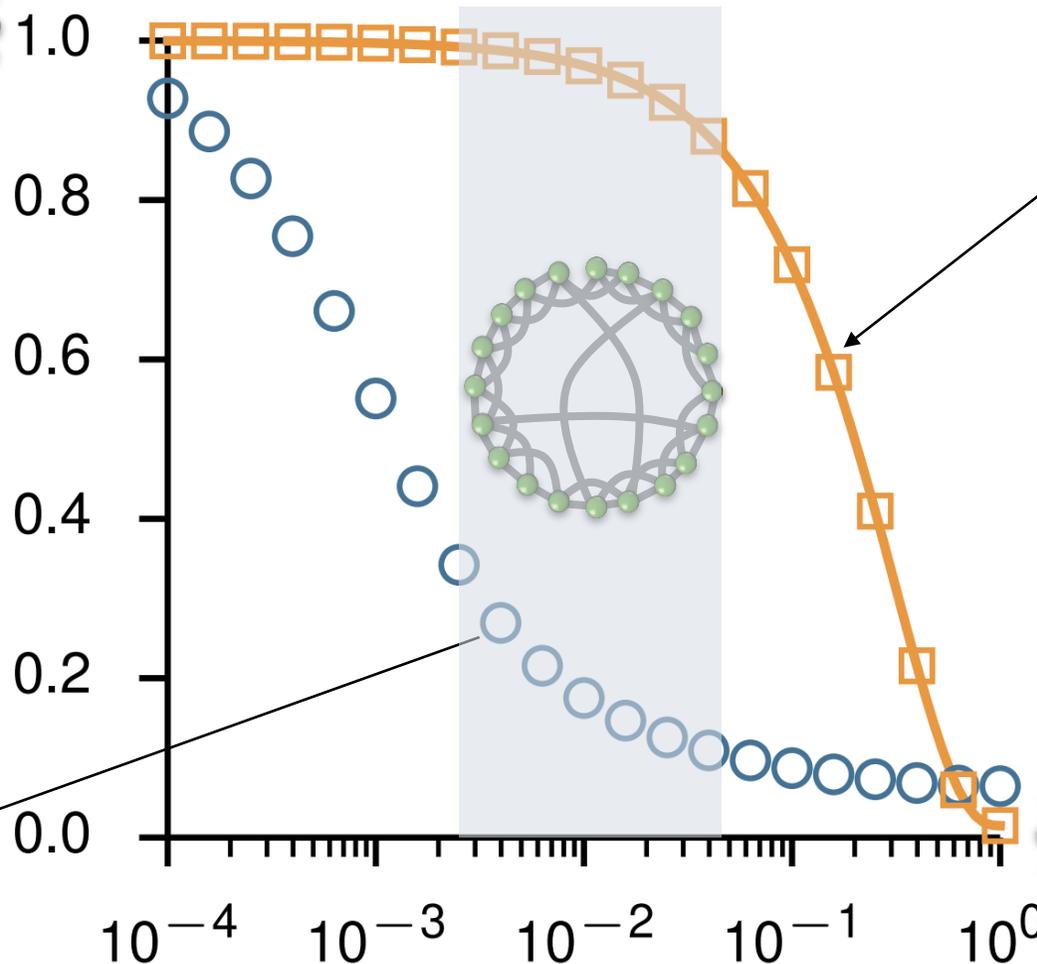


Network models

Watts-Strogatz model



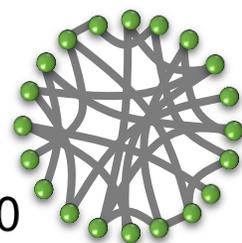
$\ell(\beta) / \ell(0), C(\beta) / C(0)$



$$\bar{C} = \frac{1}{n} \sum_i C_i$$

$$C_i = \frac{2t_i}{k_i(k_i - 1)}$$

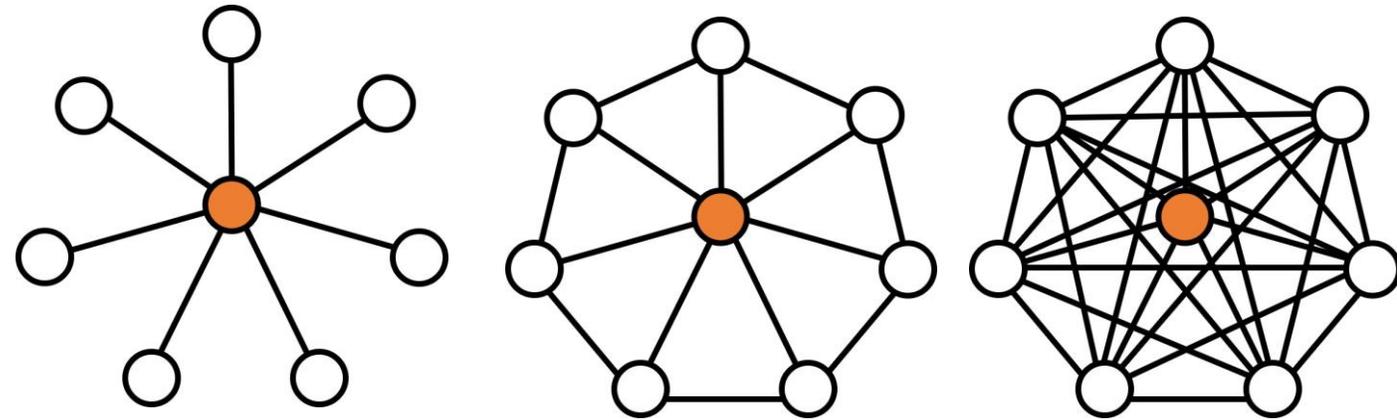
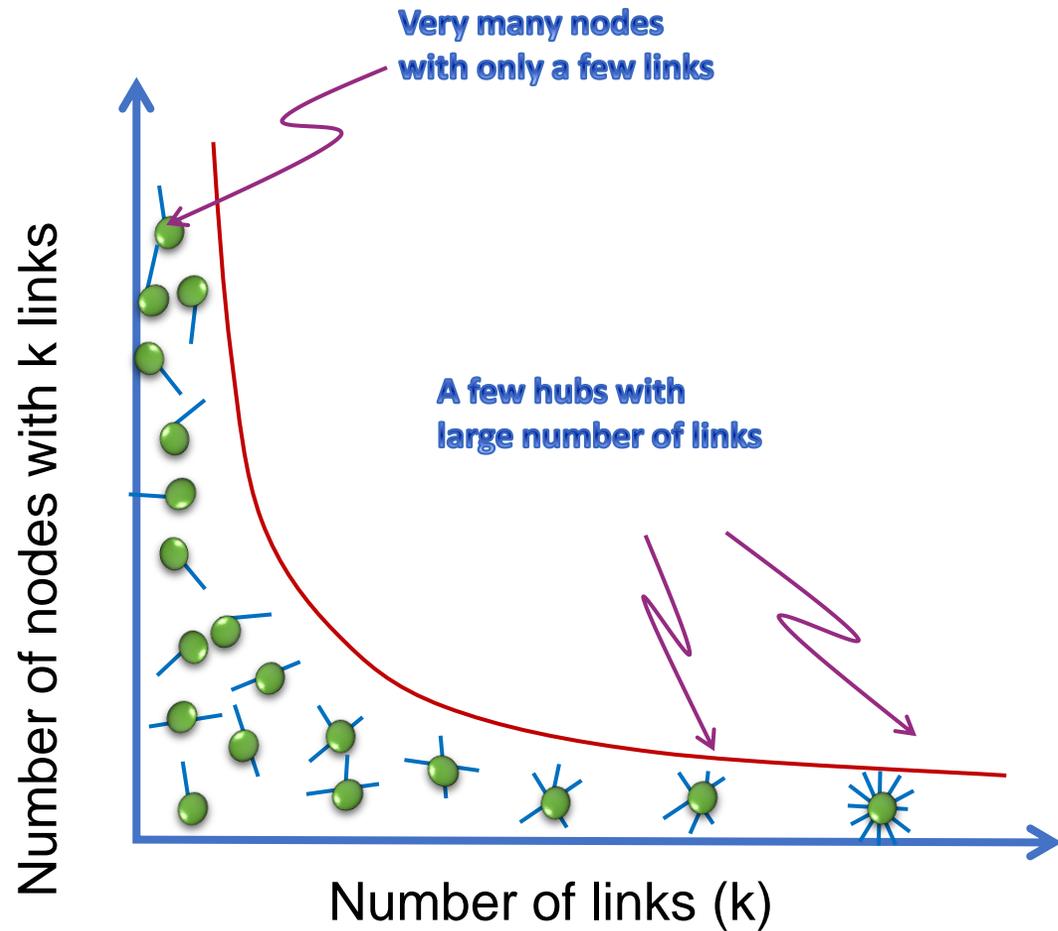
$$\bar{l} = \frac{1}{n(n-1)} \sum_{i,j} d_{ij}$$



Rewiring probability, β

Network models

Barabási-Albert model



The three \bullet nodes are equivalent in terms of the number of one-step paths connecting them to other nodes, but not in terms of the total number of routes connecting them to \circ nodes.

Definition 1. Let $G = (V, E)$ be a simple, undirected and connected graph. The matrix $A = (A_{vw})_{n \times n}$ is the *adjacency matrix* of G , and it has entries given by

$$A_{vw} = \begin{cases} 1 & \text{if } (v, w) \in E \\ 0 & \text{if } (v, w) \notin E. \end{cases}$$

Definition 2: A *walk* of length l , is any sequence of (not necessarily different) nodes v_1, \dots, v_l such as for each $i = 1, \dots, l$ there is a link from v_i to v_{i+1} . It is *closed* if $v_1 = v_l$.

Lemma 3. The number of walks of length l between the nodes v and w in a network is equal to: $(A^l)_{vw}$.

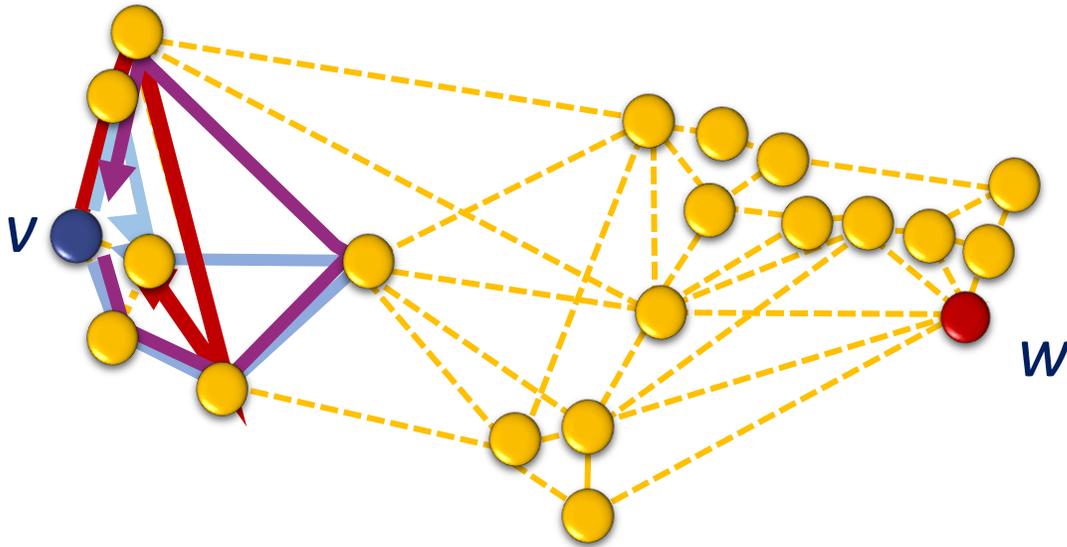
Definition 4. *The communicability function is given by the total number of walks, weighted in decreasing order of their lengths, connecting the vertices p and q in a network G*

$$G_{pq}(\zeta) = \sum_{k=0}^{\infty} \frac{(\zeta^k A^k)_{pq}}{k!} = (e^{\zeta A})_{pq}$$

where the weighting $(k!)^{-1}$ is selected among the several possibilities, and ζ is an empirical parameter.

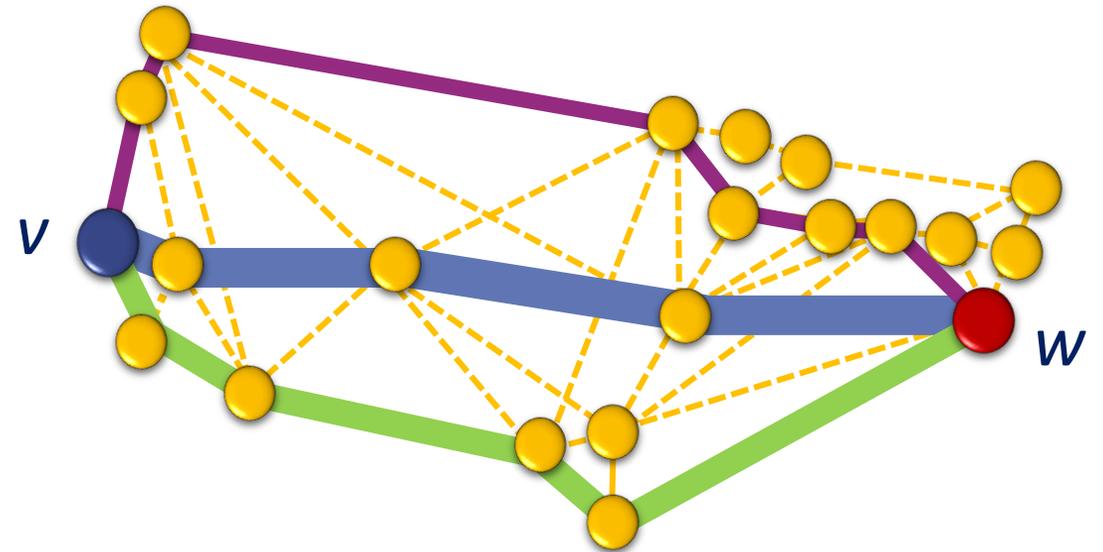
Preliminaries

$G_{vv}(\zeta)$: accounts for all walks starting and ending at the same node



It accounts for how much a **node v** retains an "item" at it, as the item goes back and forth to the node infinitely.

$G_{vw}(\zeta)$: accounts for all walks starting at v and ending at w



It accounts for how much a second node w attracts an "item" located at the node v , as the item ends up at w every time that it departs from v .

Definition 5. The “resistance” that the network offers to an “item” at node v to go to the node w is given by the difference:

$$R_{vw}(\zeta) := G_{vv}(\zeta) - G_{vw}(\zeta),$$

which is small when there are more walks “conductive” between the two nodes than those “regressive” to the origin. Hereafter $\zeta \equiv 1$ for the sake of simplicity.

Theorem 6. The inter-node resistive function

$$\xi_{vw} := R_{vw} + R_{wv} = \sum_{j=1}^n e^{\lambda_j} \left(\psi_{jv} - \psi_{jw} \right)^2$$

where ψ_{jv} is the v -th entry of the eigenvector associated with the j -th eigenvalue λ_j of A , is a squared Euclidean distance between the nodes v and w in the network and induces an embedding of the network in an n -dimensional Euclidean sphere.

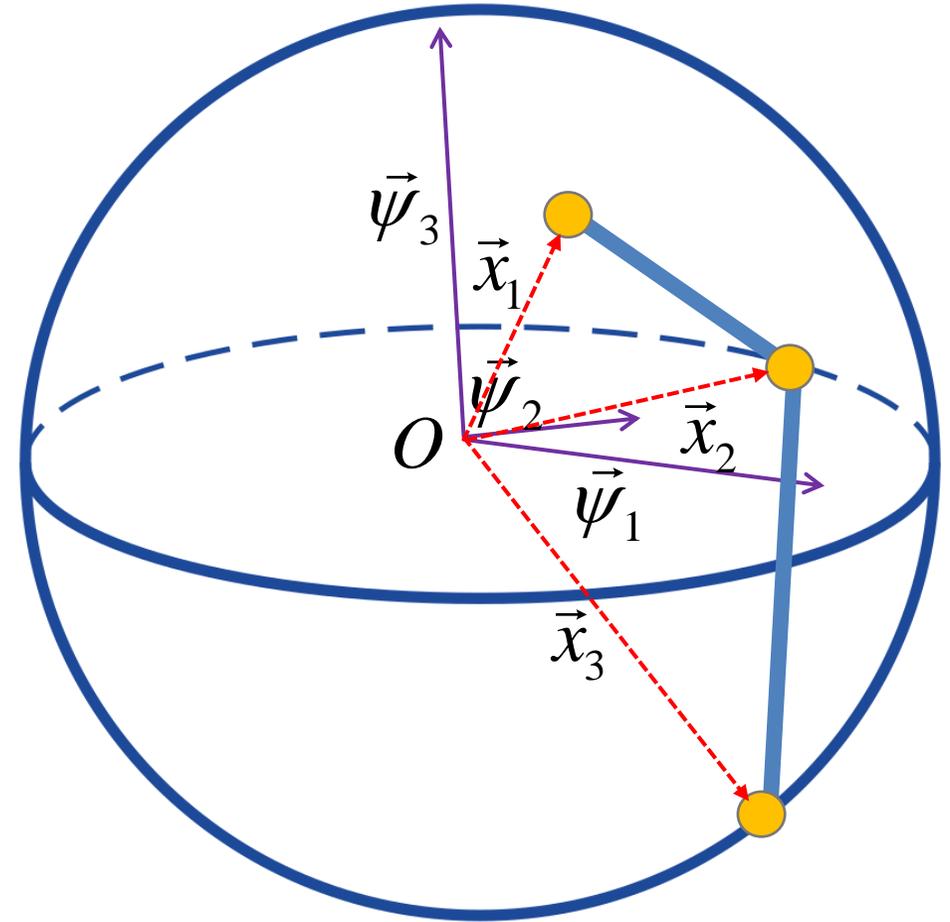
Theorem 7: *The communicability distance induces an embedding of a network into an Euclidean n -sphere*

$$S^n = \{x \in \mathbb{R}^{n+1} : \|x\| = R\}$$

where:

$$R(G) = \frac{1}{2} \sqrt{\left(\vec{s}^T e^{-A} \vec{s} - \frac{(2 - \vec{s}^T e^{-A} \vec{1})^2}{\vec{1}^T e^{-A} \vec{1}} \right)}$$

with $\vec{s} = \text{diag}(e^{\gamma A})$.



Definition 8: A matrix $\mathbf{D} = (d_{ij})$ is called Euclidean distance matrix (EDM) if there are points p^1, p^2, \dots, p^n in some Euclidean space \mathbb{R}^r such that

$$d_{ij} = \|p^i - p^j\|^2$$

for all $i, j = 1, \dots, n$, where $\| \cdot \|$ denotes Euclidean norm. If the points p^1, p^2, \dots, p^n lie on a hypersphere, then the EDM is called spherical EDM or circum-Euclidean matrix.

Therefore, $M = [\xi_{vw}]_{n \times n}$ is a circum-Euclidean distance matrix.

Lemma 9: M is non singular and

$$M^{-1} = -\frac{1}{2}e^{-A} + \frac{caa^T - (\varepsilon - 2)b^T a^T - (\varepsilon - 2)ab + db^T b}{2(cd - (\varepsilon - 2)^2)}$$

where $a = e^{-A}\mathbf{1}$, $b = s^T e^{-A}$, $c = s^T e^{-A}s$, $d = \mathbf{1}^T e^{-A}\mathbf{1}$, $\varepsilon = s^T e^{-A}\mathbf{1}$ and $s = \text{diag}(e^A)$.

Proof:

- Use the Sherman-Morrison-Woodbury formula;
- Show that $cd - (\varepsilon - 2)^2 \neq 0$;
- It can also be shown that $\mathbf{1}^T M^{-1}\mathbf{1} \neq 0$ as required for circum-EDM.

Lemma 10: Let $\mathcal{L} := e^{-A} - \frac{aa^T}{d}$. Then, \mathcal{L} is the unique Laplacian matrix associated with the matrix M of the graph.

Proof:

- Use a result of Balaji and Bapat about nonsingular spherical EDM and Laplacians to find that

$$M^{-1} = -\frac{1}{2} \mathcal{L} + \frac{M^{-1} \mathbf{1} \mathbf{1}^T M^{-1}}{\mathbf{1}^T M^{-1} \mathbf{1}}$$

- Find $M^{-1} \mathbf{1} \mathbf{1}^T M^{-1}$.

Theorem 11: Let \mathcal{L} be the Laplacian matrix associated with the matrix M of the graph. Then,

$$M = \rho \mathbf{1}^T + \mathbf{1} \rho^T - 2\mathcal{L}^+$$

where

$$\mathcal{L}^+ = e^A + \left(\frac{\mathbf{1}^T e^A \mathbf{1}}{n^2} \right) \mathbf{1} \mathbf{1}^T - \frac{1}{n} \left(\mathbf{1} \mathbf{1}^T e^A + e^A \mathbf{1} \mathbf{1}^T \right)$$

is the Moore-Penrose pseudoinverse of \mathcal{L} , and $\rho = \text{diag}(\mathcal{L}^+)$.

Proof: We use the fact that

$$\mathcal{L}^+ = \left(\mathcal{L} + \frac{1}{n} \mathbf{1}\mathbf{1}^T \right)^{-1} - \frac{1}{n} \mathbf{1}\mathbf{1}^T.$$

Let us write

$$\left(\mathcal{L} + \frac{1}{n} \mathbf{1}\mathbf{1}^T \right)^{-1} = \left(e^{-A} + \frac{1}{n} \mathbf{1}\mathbf{1}^T - \frac{aa^T}{d} \right)^{-1},$$

and apply twice the Sherman-Morrison-Woodbury formula to obtain

$$\left(\mathcal{L} + \frac{1}{n} \mathbf{1}\mathbf{1}^T \right)^{-1} = e^{-A} - \frac{ff^T}{n + g},$$

where $f = e^A \mathbf{1}$ and $g = \mathbf{1}^T e^A \mathbf{1}$.

We then obtain

$$\left(\mathcal{L} + \frac{1}{n} \mathbf{1}\mathbf{1}^T \right)^{-1} = e^A + \left(\frac{n+g}{n^2} \right) \mathbf{1}\mathbf{1}^T - \frac{1}{n} (\mathbf{1}f^T + f\mathbf{1}^T).$$

Therefore,

$$\left(\mathcal{L} + \frac{1}{n} \mathbf{1}\mathbf{1}^T \right)^{-1} - \frac{1}{n} \mathbf{1}\mathbf{1}^T = e^A + \left(\frac{g}{n^2} \right) \mathbf{1}\mathbf{1}^T - \frac{1}{n} (\mathbf{1}\mathbf{1}^T e^A + e^A \mathbf{1}\mathbf{1}^T).$$

We now prove that $M = \rho\mathbf{1}^T + \mathbf{1}\rho^T - 2\mathcal{L}^+$. First, let $T_i := \sum_{j=1}^n (e^A)_{ij}$ be the total communicability of node i . Then,

$$\mathcal{L}_{ij}^+ = (e^A)_{ij} + \frac{g}{n^2} - \frac{1}{n} (T_i + T_j).$$

Thus

$$\begin{aligned}\mathcal{L}_{ii}^+ + \mathcal{L}_{jj}^+ - 2\mathcal{L}_{ij}^+ &= \left(e^A\right)_{ii} + \frac{g}{n^2} - \frac{2T_i}{n} + \left(e^A\right)_{jj} + \frac{g}{n^2} - \frac{2T_j}{n} - 2\left(\left(e^A\right)_{ij} + \frac{g}{n^2} - \frac{T_i + T_j}{n}\right) \\ &= \left(e^A\right)_{ii} + \left(e^A\right)_{jj} - 2\left(e^A\right)_{ij} \\ &= M_{ij}.\end{aligned}$$

Definition 12: The *effective resistance* between two nodes $i, j \in \{1, \dots, n\}$ of a graph with Laplacian L is given by

$$R_{ij} = (e_i - e_j)^T L^+ (e_i - e_j)$$

where L^+ is the pseudoinverse of L . The effective resistance matrix $R = [R_{ij}]$ is defined as

$$R = r\mathbf{1}\mathbf{1}^T + \mathbf{1}\mathbf{1}^T r - 2L^+$$

where $r = \text{diag}(L^+)$.

The square root of R_{ij} is metric, and R is a Euclidean distance matrix, i.e., it has nonnegative elements, zero diagonal and it is negative semidefinite on $\mathbf{1}^\perp$.

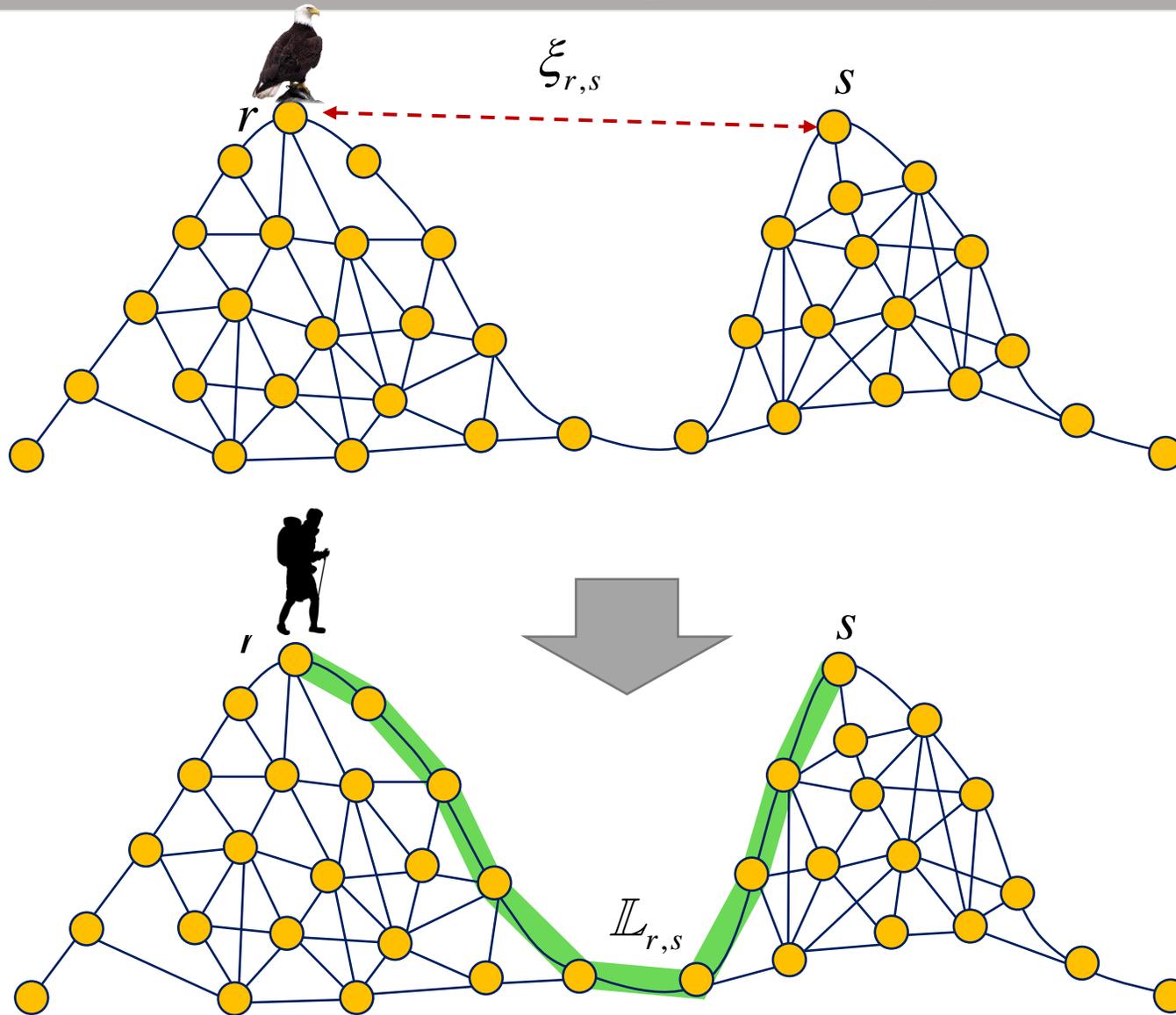
Remark 13. *The communicability distance between two nodes $i, j \in \{1, \dots, n\}$ of a graph can be expressed as*

$$\xi_{ij} = (e_i - e_j)^T \mathcal{L}^+ (e_i - e_j)$$

and represents an effective resistance between them when the edges of the graph are weighted in a specified way.

Corollary 14. *Let Ξ be any nonsingular circum-EDM. Then, Ξ is a resistance EDM of the graph with the edges appropriately weighted.*

Communicability geometry

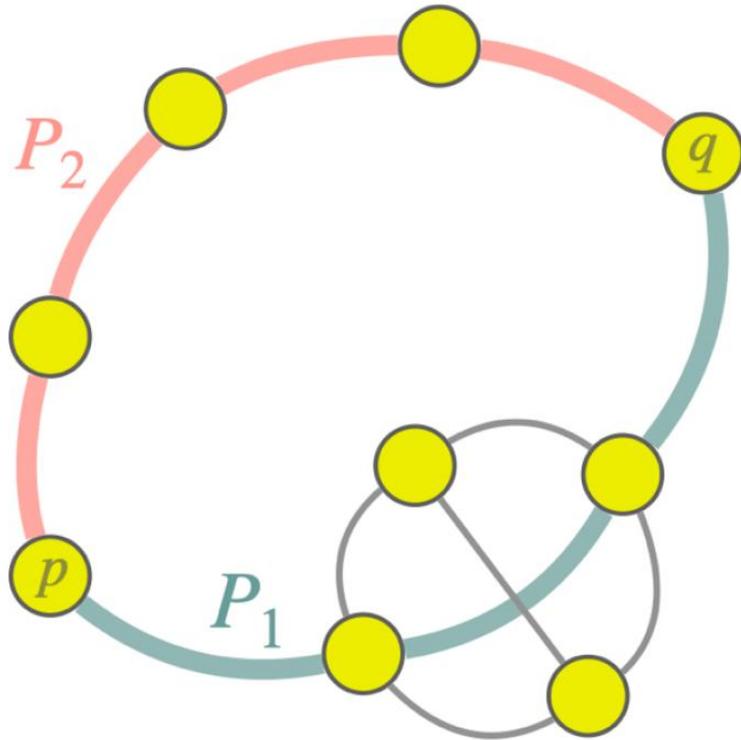


Geometrization: consider every edge $e=pq$ in E as a compact 1-dimensional manifold with boundary $\partial e = p \cup q$. Let the edge $e=pq$ be given the metric $\mathbb{L}_{p,q}$, such that

$$\tilde{e}_{pq} \underset{\text{isom}}{\cong} \begin{cases} [0, \xi_{pq}] & (p, q) \in E, \\ 0 & (p, q) \notin E. \end{cases}$$

Extend the distance metric $\mathbb{L}_{p,q}$ on the edges of G via infima of lengths of curves in the geometrization of G . Then, the graph becomes metrically length spaces. This space is *locally compact, complete and geodesic*.

Definition 15. Let $p(v \rightarrow w)$ be a path between the nodes v and w in G . The *communicability resistive path length* is defined as the sum of $\mathbb{L}_{p,q}$ for all edges in the path. Hereafter, $\mathbb{L}_{p,q}$ will be called *resistive path length*.



Path lengths

topological

$$l(P_1) = 3$$

$$l(P_2) = 4$$

electric

$$\mathbb{R}(P_1) = 2.15$$

$$\mathbb{R}(P_2) = 3.38$$

Edge resistive length

Let $\mathbb{L}_{SP}(v, w)$ be the resistive length of the topological SP. Let $\mathbb{L}_{SRP}(v, w)$ be the length of the shortest resistive path (SRP) between the same pair of nodes. Then,

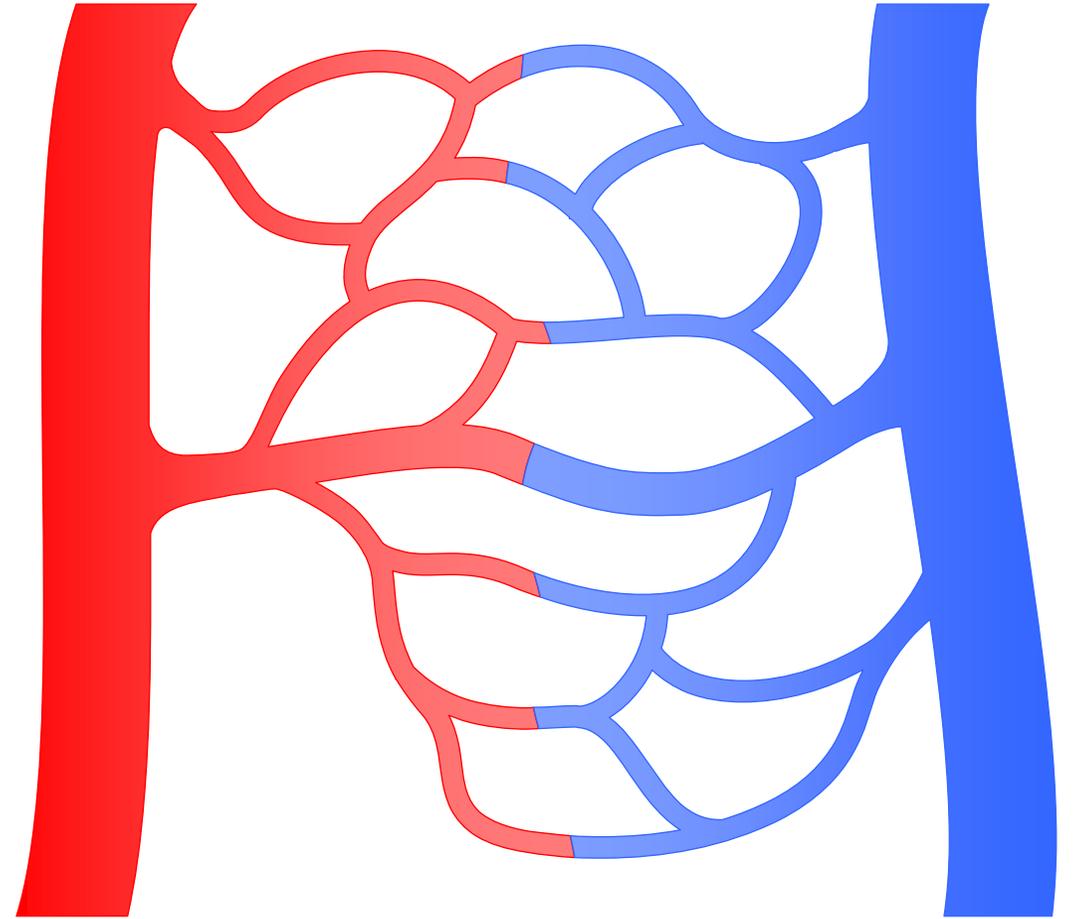
$$\mathbb{L}_{SRP}(v, w) \leq \mathbb{L}_{SP}(v, w).$$

When, $\mathbb{L}_{SRP}(v, w) < \mathbb{L}_{SP}(v, w)$ we call SRP a *bypass* between the nodes v and w .

Bypasses in nature

*“The collateral circulation is a **network** of specialized endogenous **bypass** vessels that is present in most tissues and **provides protection** against ischemic injury caused by ischemic stroke, coronary atherosclerosis, peripheral artery disease, and other conditions and diseases.”*

Faber et al.: *Arterioscler Thromb Vasc Biol.* 34 (2014) 1854-1859.



Edge resistive length

Let $\bar{L}_{SP}(e)$ be the *mean edge resistive length* along the SP, and let $\bar{L}_{SRP}(e)$ be the same along the SRP. Obviously,

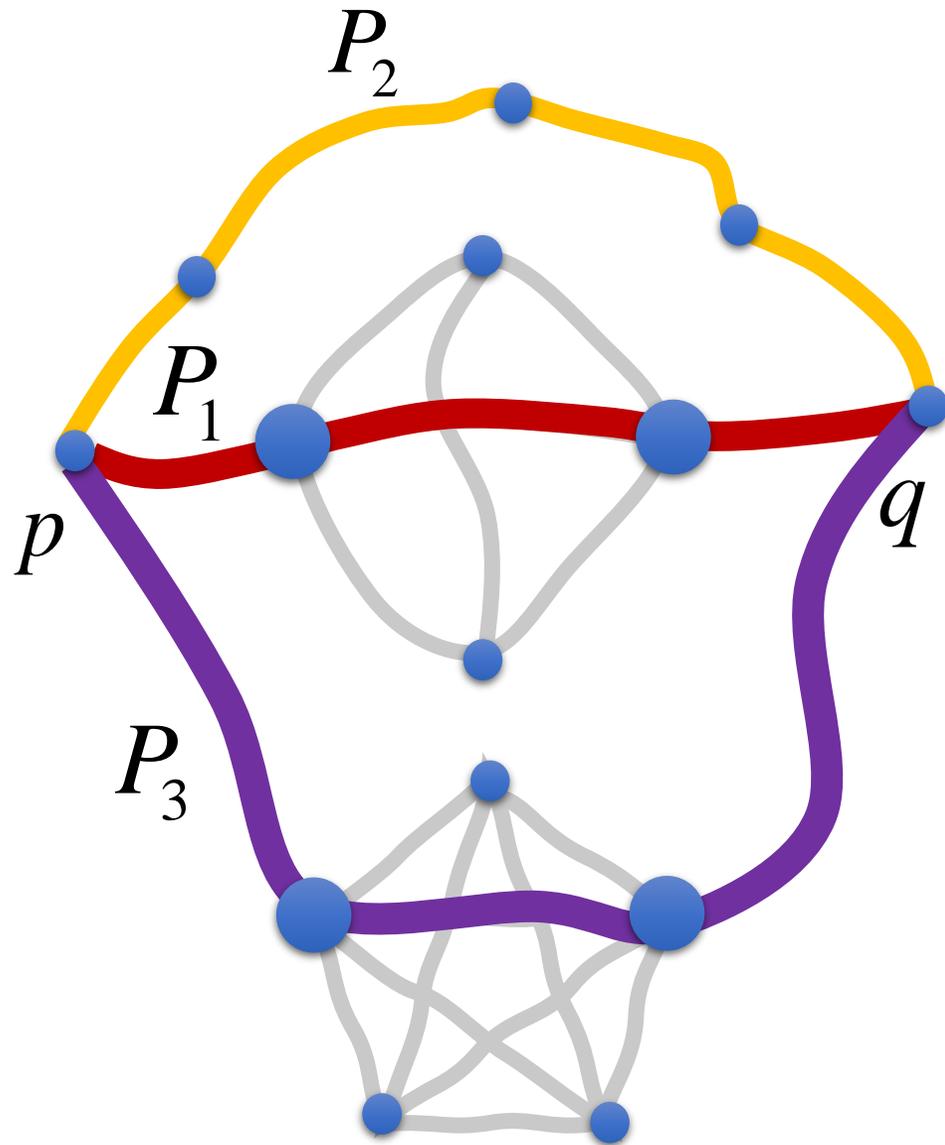
$$\bar{L}_{SRP}(e) \cdot l_{SRP} \leq \bar{L}_{SP}(e) \cdot l_{SP}$$

Therefore,

$$\tilde{\varepsilon} := \frac{l_{SP}}{l_{SRP}} \geq \frac{\bar{L}_{SRP}(e)}{\bar{L}_{SP}(e)}$$

is an *upper bound* to the ratio of the mean edge resistive length in the SRP relative to that of the SP.

Why to use the bound?

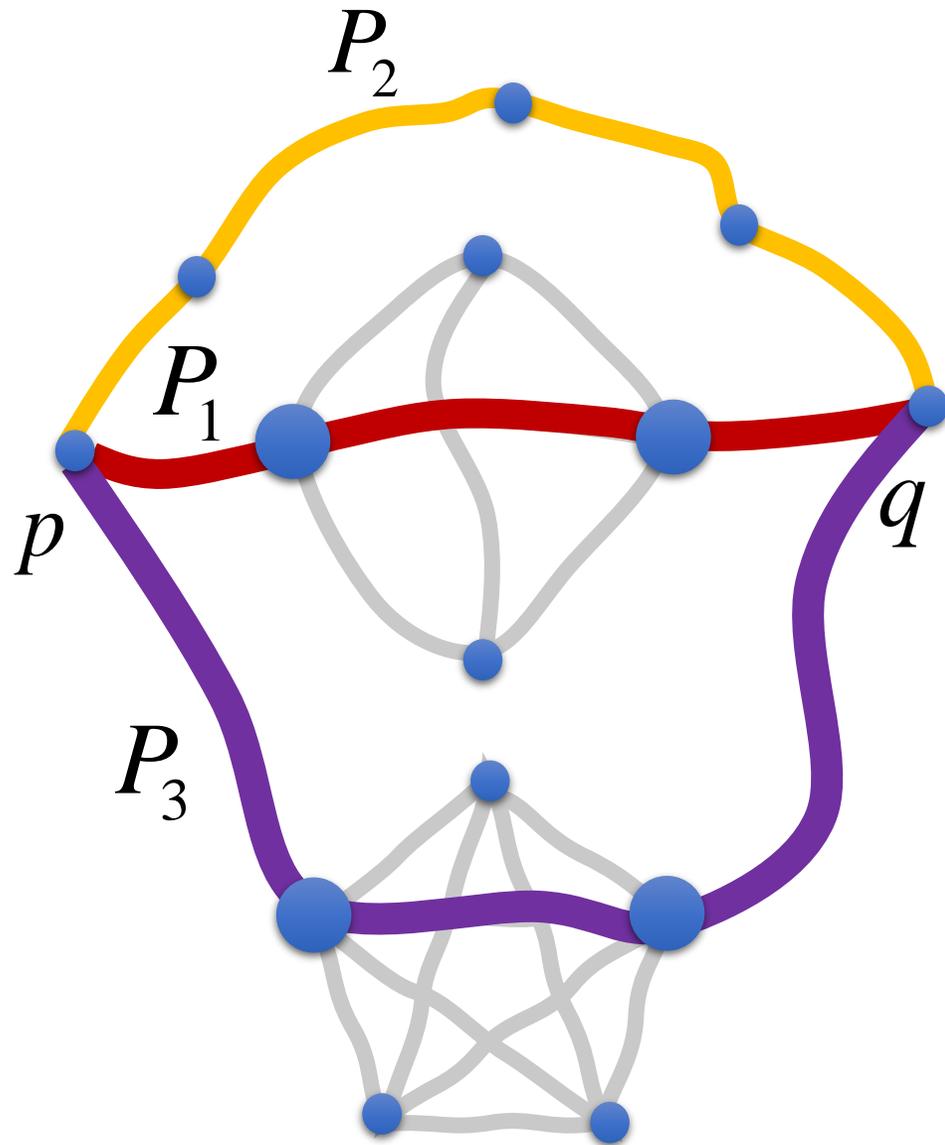


- 1) Identify all shortest paths between the two nodes;
- 2) Identify the shortest resistive path;
- 3) Calculate $\bar{\mathbb{L}}_{SRP}(e) / \bar{\mathbb{L}}_{SP}(e)$ for every SP.

$$\frac{\bar{\mathbb{L}}_{P_2}(e)}{\bar{\mathbb{L}}_{P_1}(e)} \approx 0.7444$$

$$\frac{\bar{\mathbb{L}}_{P_2}(e)}{\bar{\mathbb{L}}_{P_3}(e)} \approx 0.5739$$

Why to use the bound?



- 1) Identify ONE shortest paths between the two nodes;
- 2) Identify THE shortest resistive path;
- 3) Calculate l_{SP} / l_{SRP} :

$$3 / 4 = 0.75$$

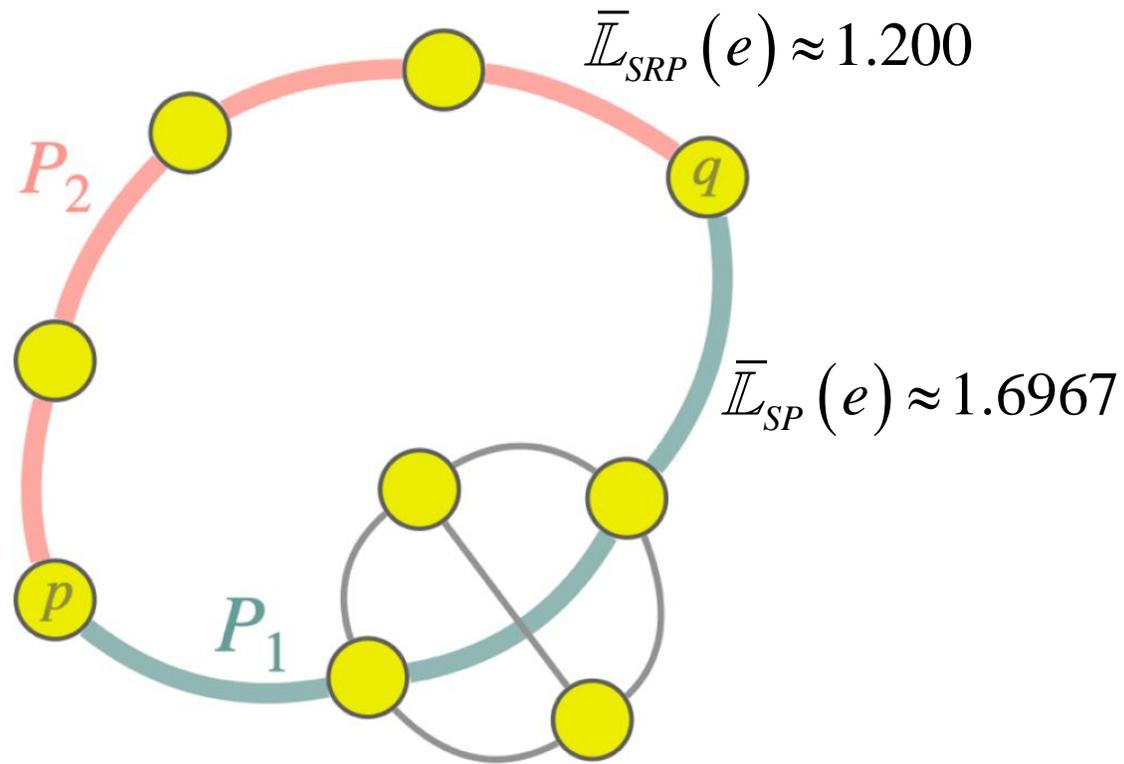
Definition 16. *Let*

$$\varepsilon_{bf}(s, t) := 100 \left(\frac{l_{SP}(s, t)}{l_{SRP}(s, t)} - 1 \right)$$

be the least percentage of “energy” that an “item” traveling between the nodes s and t can save per edge as a result of selecting the SRP instead of the SP. The average of this quantity across all possible pairs of nodes in the network is

$$\varepsilon = \left\langle \varepsilon_{bf}(s, t) \right\rangle$$

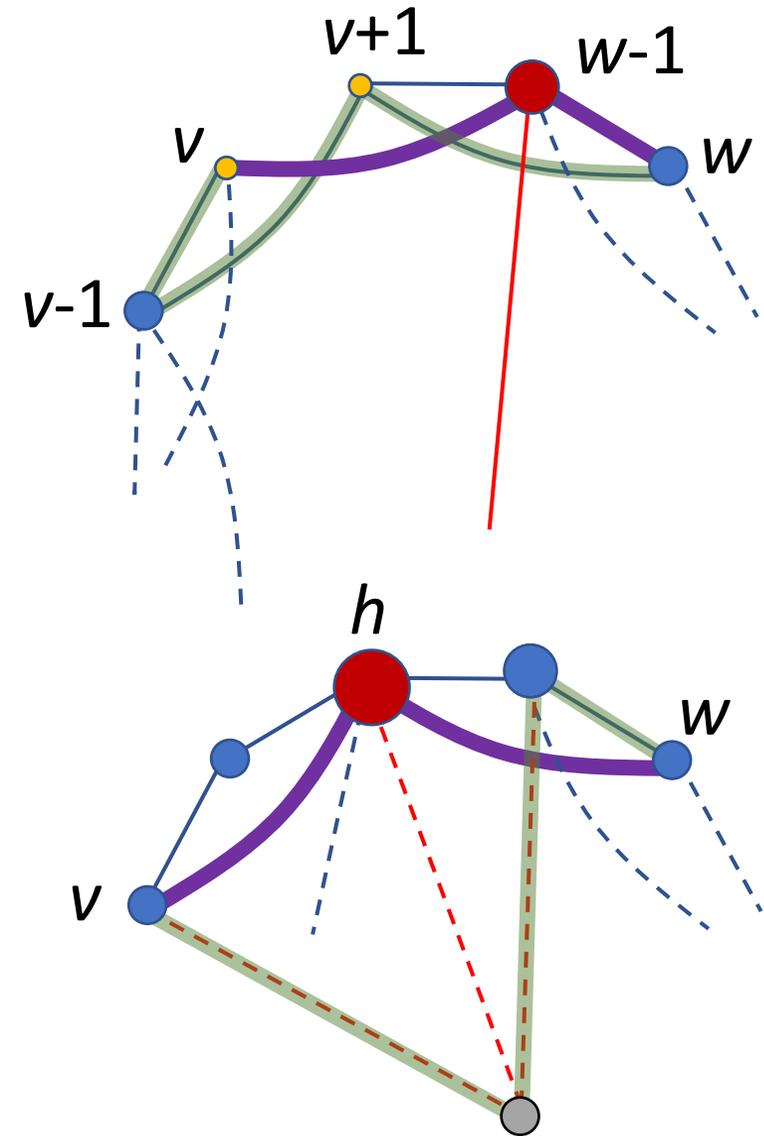
Theoretical model in a nutshell



$$\frac{\bar{L}_{SRP}(e)}{\bar{L}_{SP}(e)} \approx 0.7073$$

$$\varepsilon = 100(3/4 - 1) = -25\%$$

Back to the models



$$q_{vw} = \frac{G_{vw}}{\sum_{i < j} G_{ij}}$$

all weighted walks between v and w

all weighted walks between every pair of nodes in the network

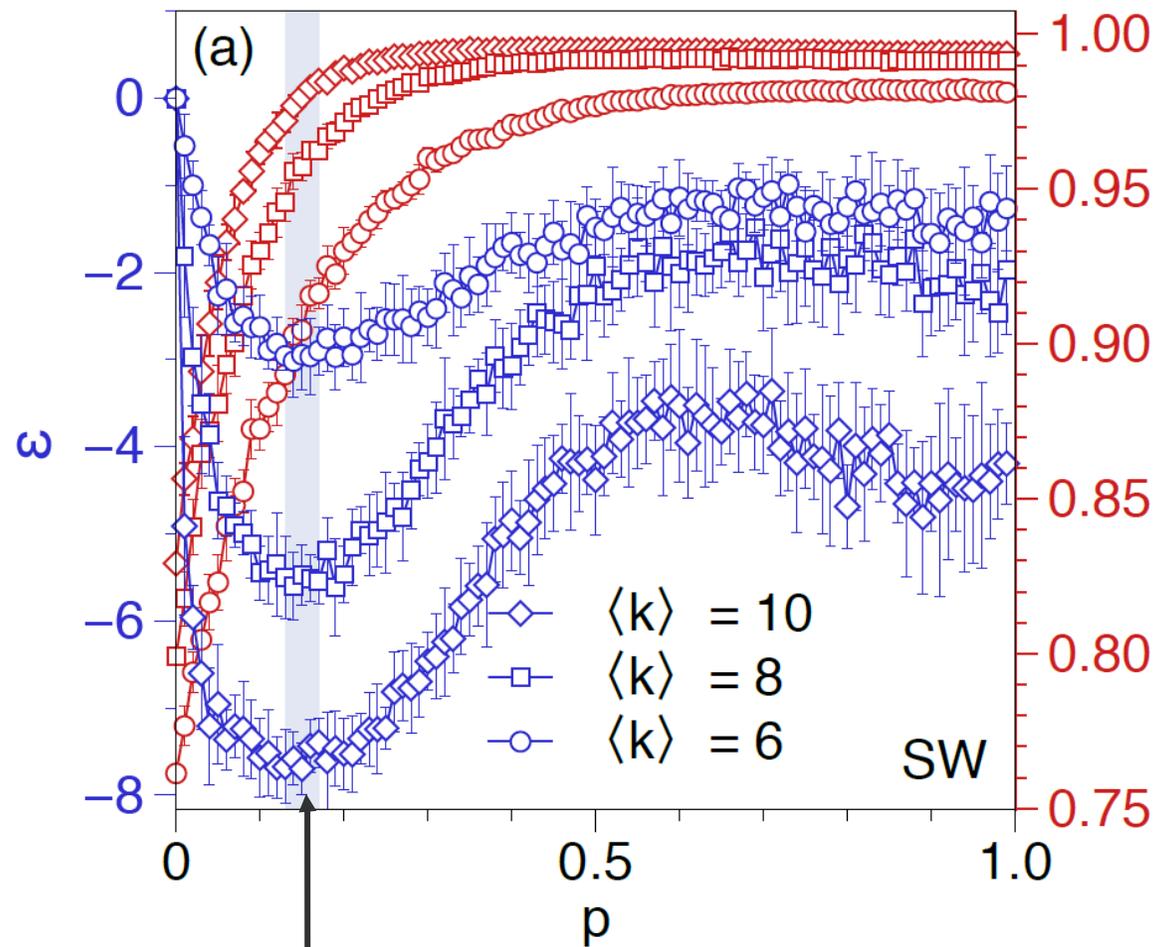
Walk Richness

$$S(q) = -\frac{1}{2} \sum_{v < w} q_{vw} \ln q_{vw}$$

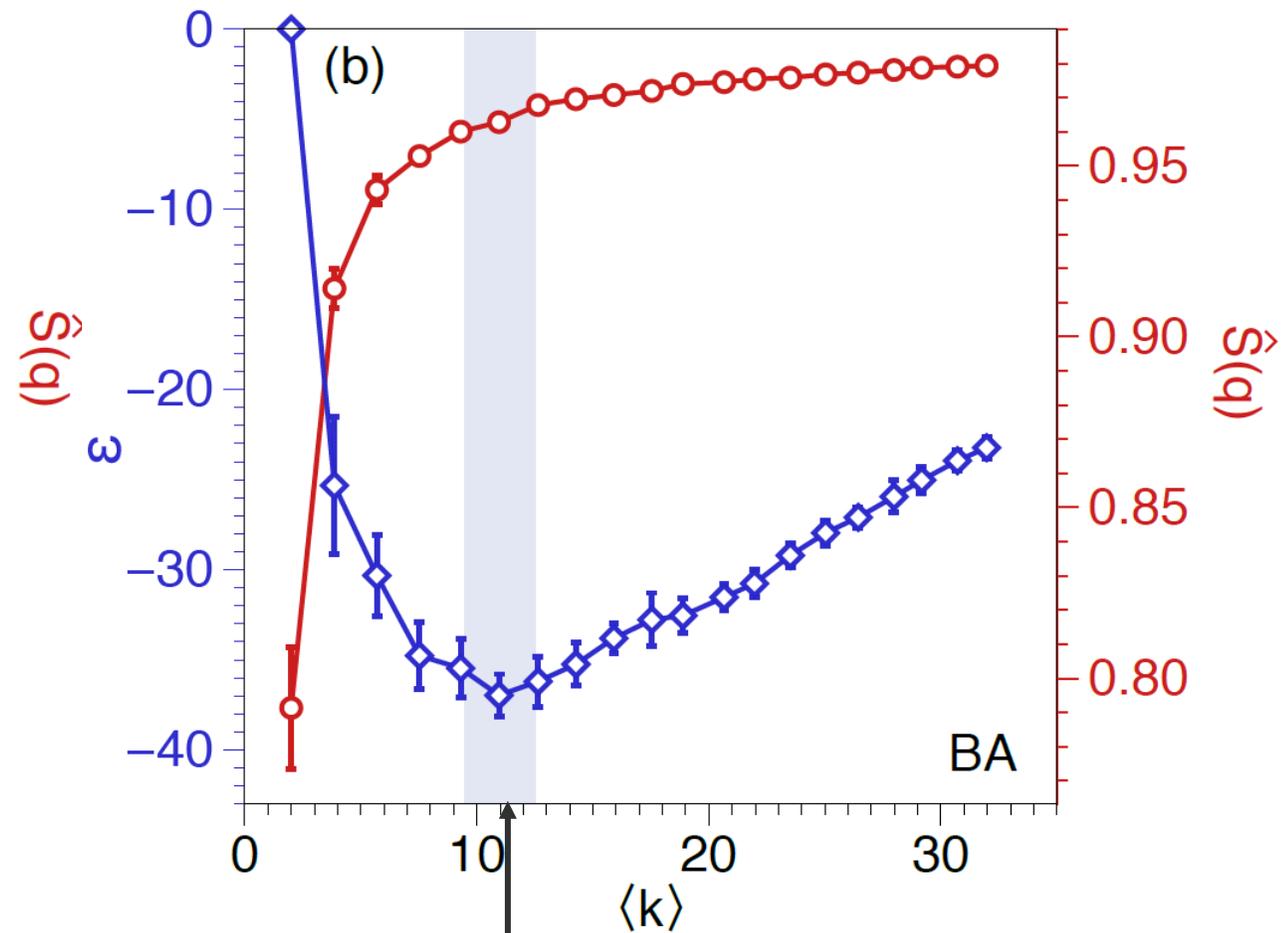
$$0 \leq \hat{S}(q) = \frac{S(q)}{\ln(n(n-1)/2)} \leq 1$$

Back to the models

Watts-Strogatz model



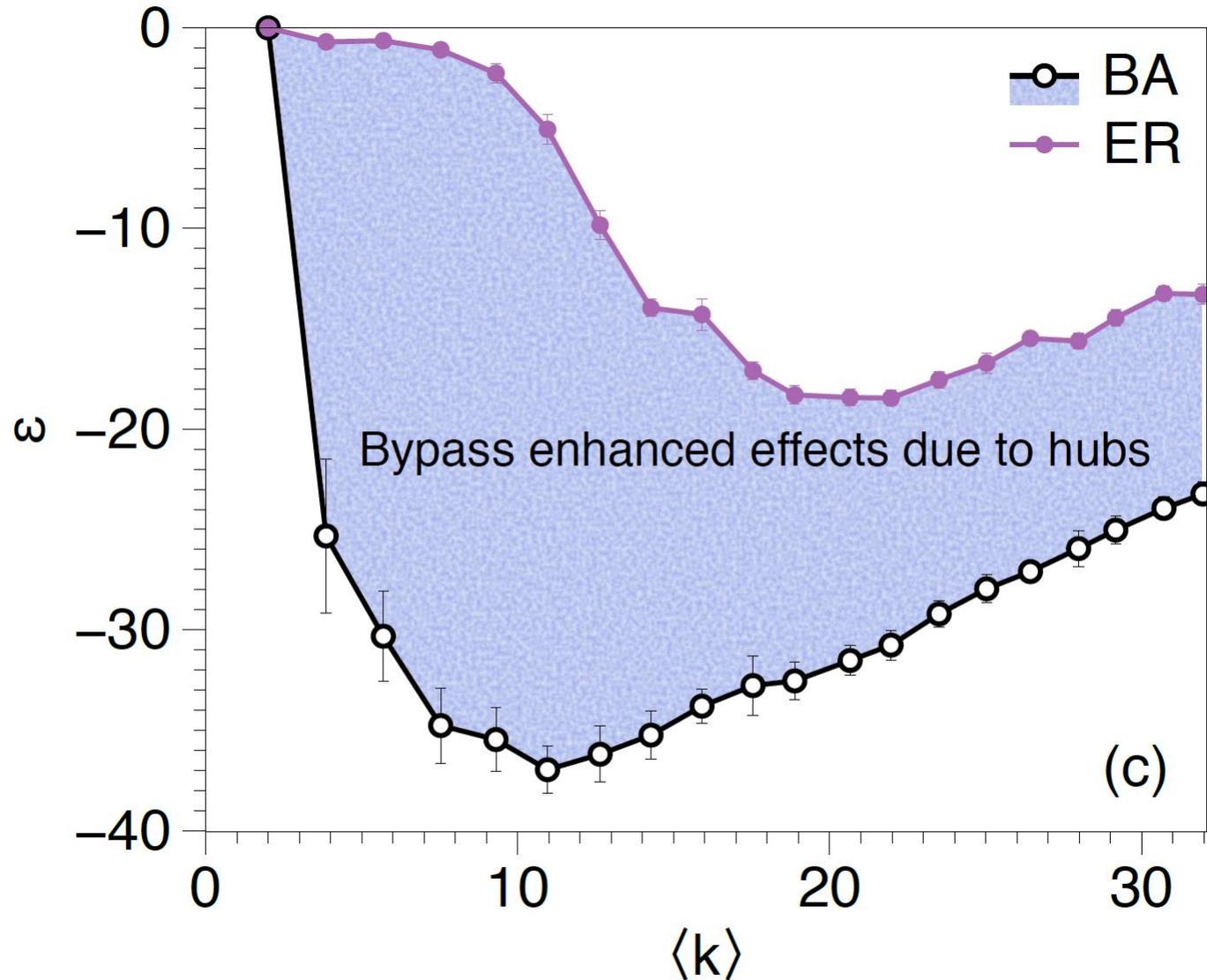
Barabási-Albert model



Good navigational point
(GNP)

- *Both processes (WS and BA) create enough walk richness as for certain bypasses among pairs of nodes EMERGE. Such bypasses avoid naturally the hubs of the network, allowing “items” navigating them to save “energy” in relation to what it will cost to navigate through the shortest paths.*

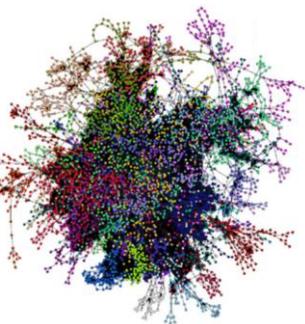
Back to the models



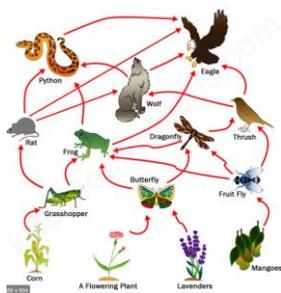
The hubs created by the PA mechanism enhance the emergence of efficient bypasses in relation to networks with more “normal-like” degree distributions.

What happen in the real-world?

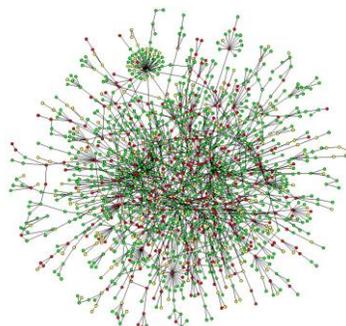
USA western power grid



Food webs



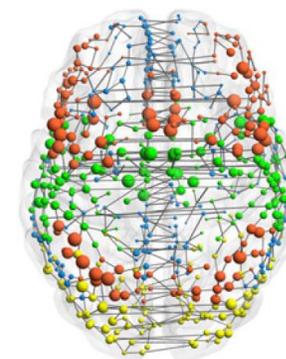
Yeast PPI network



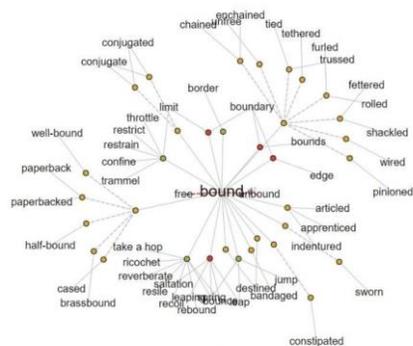
Collaboration networks



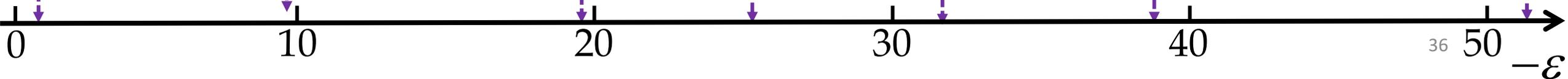
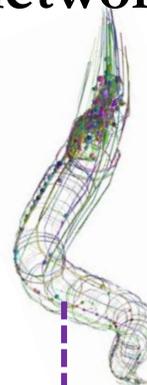
Brain functional coactivation



Roget thesaurus

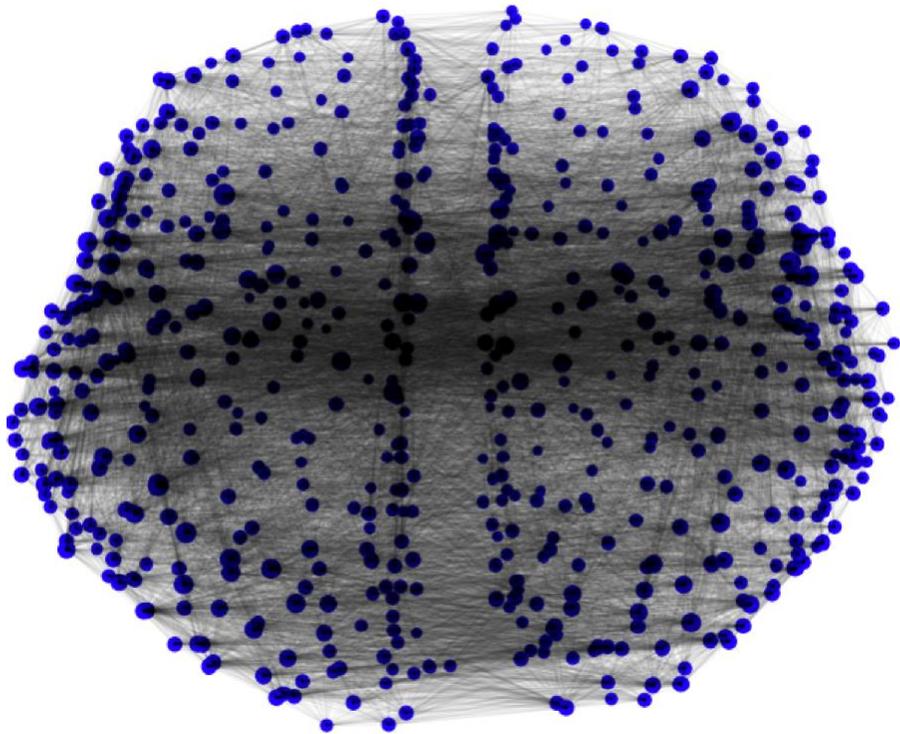


C. elegans neural network

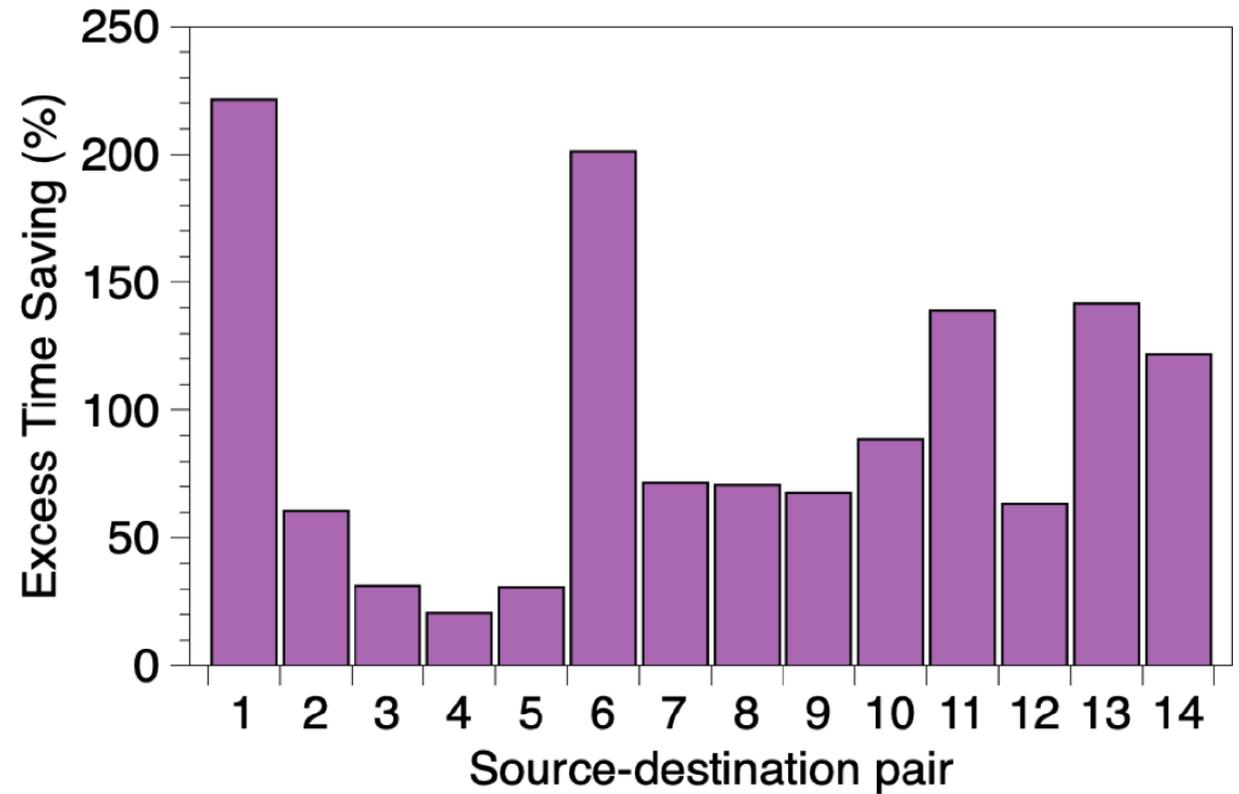


What happen in the real-world?

Brain functional coactivation



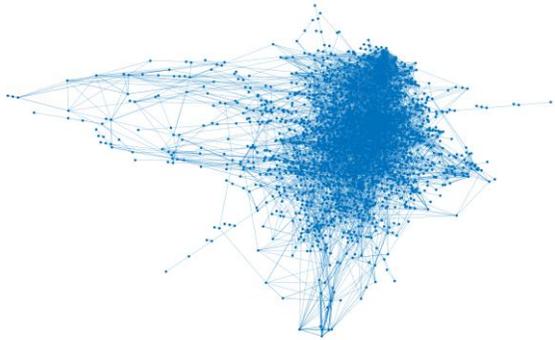
Time saving in diffusive processes



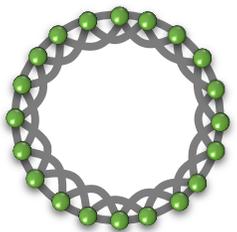
Dissimilarity between two networks

$$D(G, G') = \sqrt{\sum_{j=1}^n (\lambda_j(G) - \lambda_j(G'))^2}$$

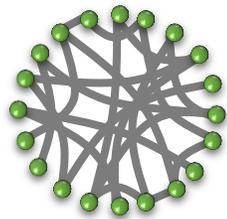
Collaboration network QcGr



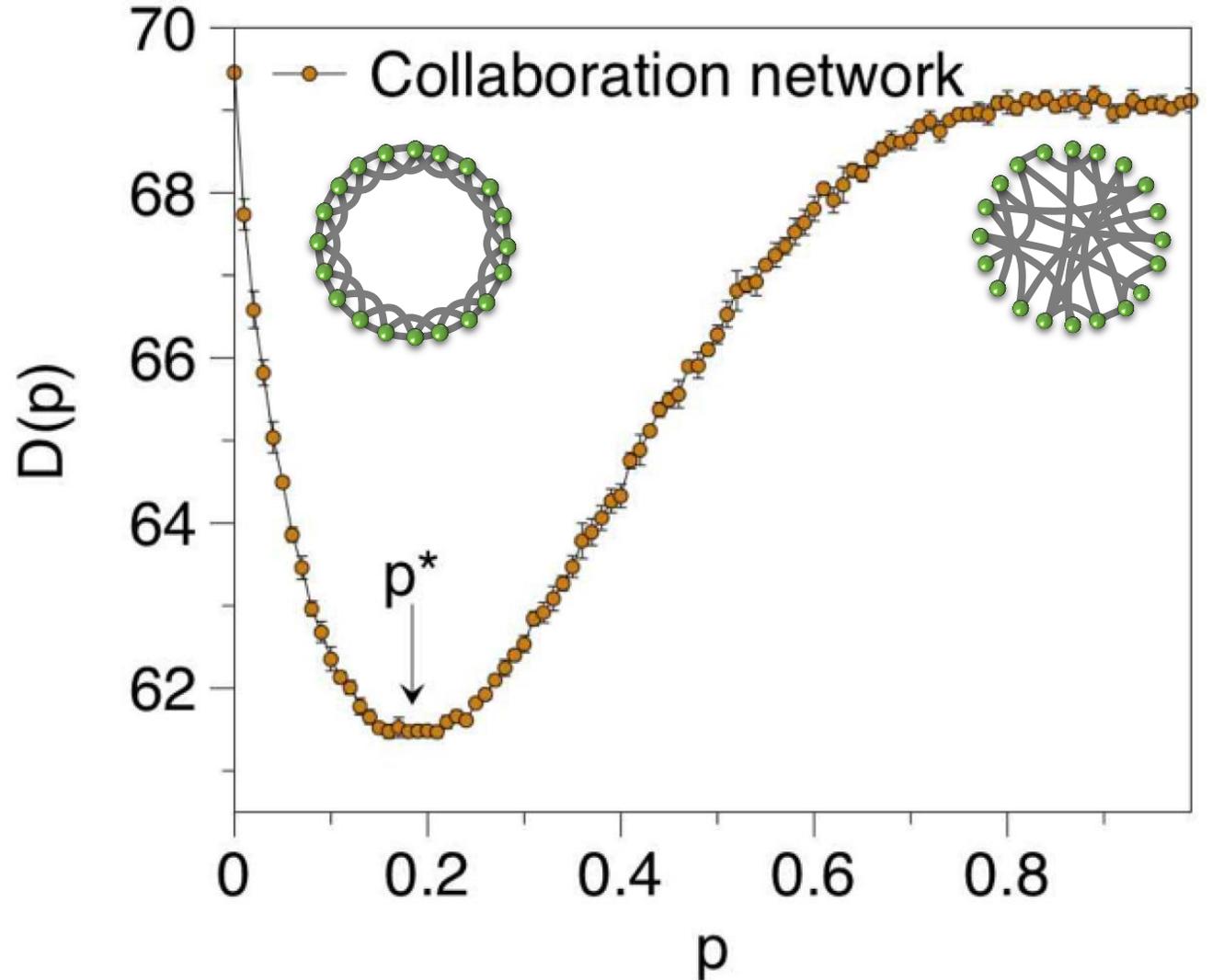
$n = 4158$
 $m = 13,422$



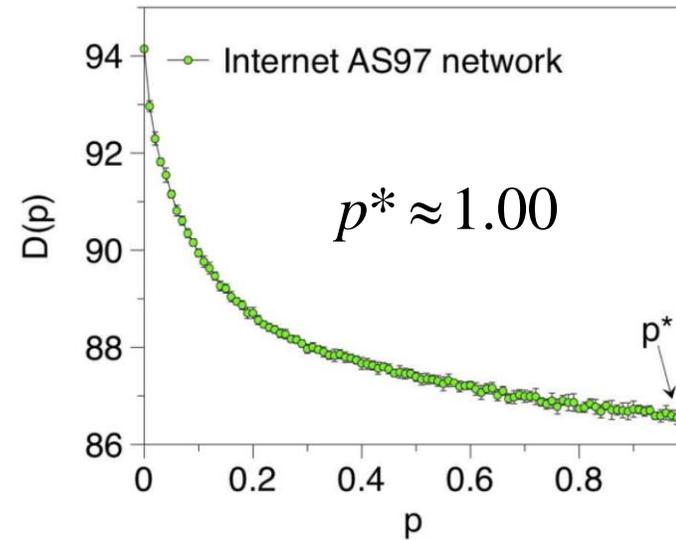
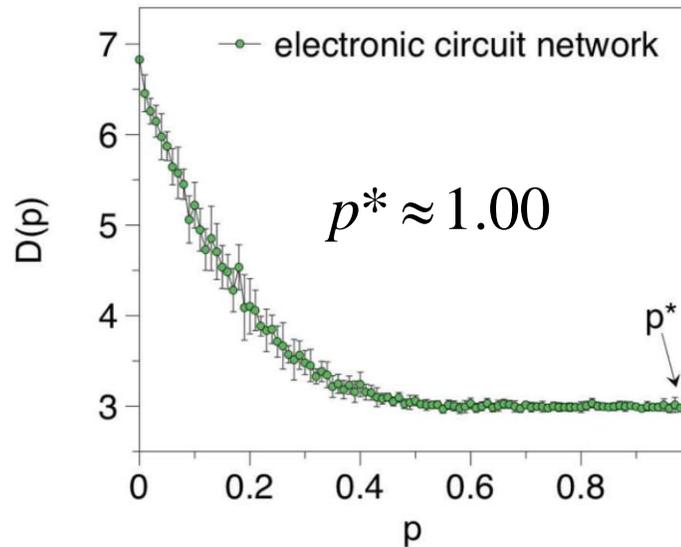
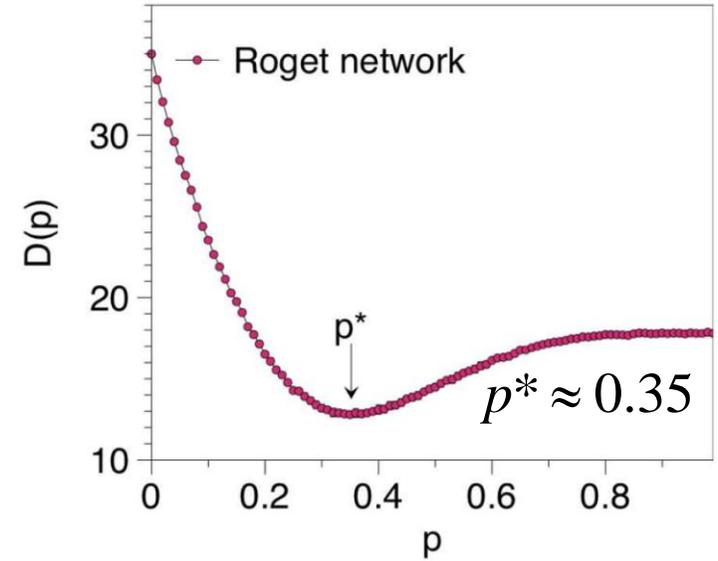
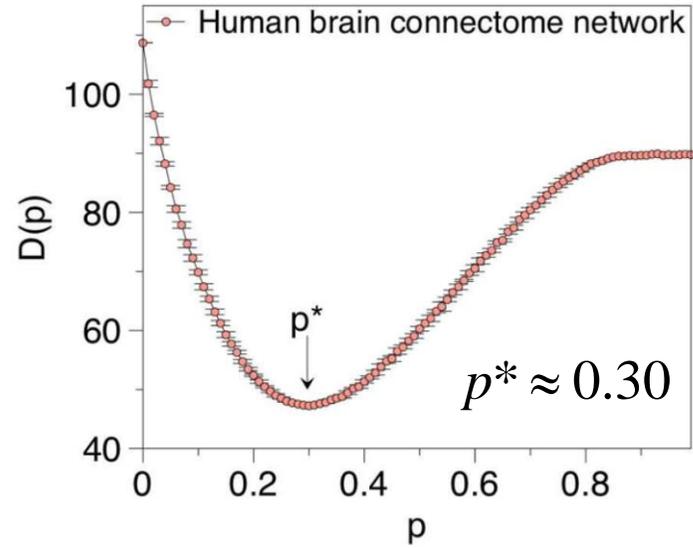
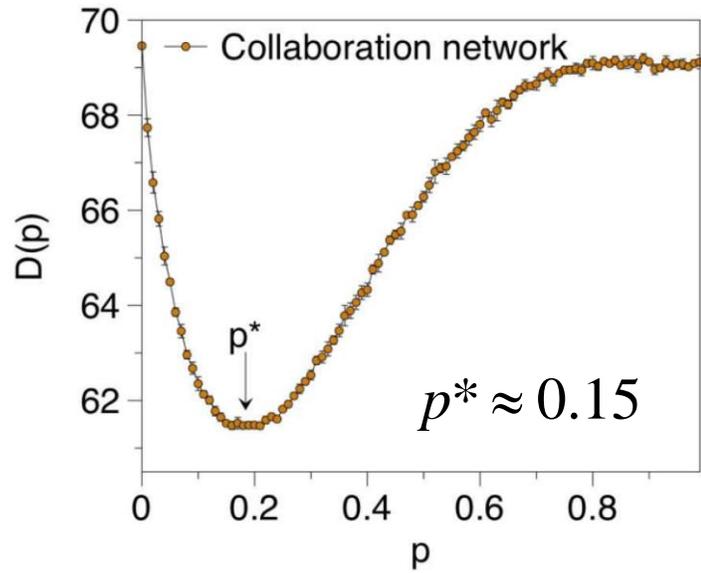
p



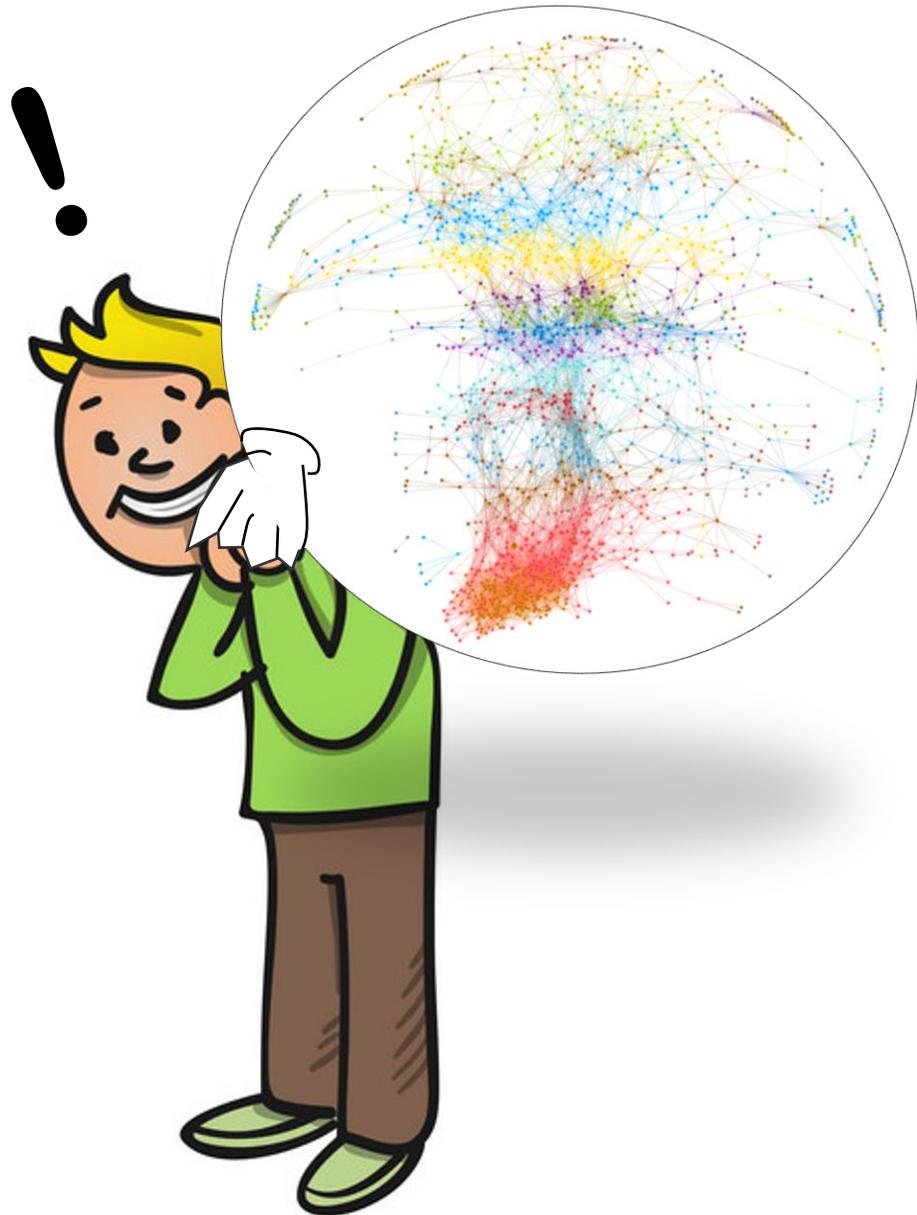
$n = 4158$
 $m = 13,422$



Real-world networks and GNP



What makes a network “complex”?



A network is said to be complex if it contains enough walk richness as for bypasses emerge as alternative best communication routes between pairs of nodes.

Simply put, bypasses seems to sustain complexity.

¿Qué tienen en común nuestras redes sociales, la coordinación muscular, el envejecimiento de nuestros órganos, nuestras células y sus componentes moleculares, la forma en que pensamos, nuestra inteligencia, el tráfico en nuestras ciudades o la basura que generamos a diario? Este libro es un recorrido por los sistemas complejos, tales como nuestros órganos y células, nuestras redes sociales, la organización de nuestras ciudades o las relaciones comerciales y geopolíticas entre los países del mundo. A merced de las redes es una peregrinación cultural, científica y humanística, a través de las redes de interdependencias que forman las entidades constituyentes de estos sistemas. Es, además de una perspectiva científica de las propiedades generales que hacen únicas y funcionales a estas redes, un acercamiento humanístico al tema, que incluye inmersiones en la pintura y la literatura, la historia, la filosofía, las ciencias sociales y políticas.

Esta aventura literaria nos hace reflexionar sobre por qué nos parece que el mundo es un «pañuelo», que haya gente más “popular” que otra, que nuestros amigos tengan más amigos que nosotros, que haya buenos y malos líderes en un grupo, que podamos coordinar nuestros movimientos o que una persona mayor pueda envejecer siendo creativa, entre otras cuestiones de nuestro día a día. Pero también nos enseña como estas mismas redes nos exponen a la propagación de una infección viral o a ser víctimas de la desinformación, a que existan atascos de tráfico en las ciudades, retrasos y cancelaciones de vuelos y de que algunas actividades humanas tengan un gran impacto medioambiental.

Enfermedades como el cáncer, los infartos cerebrales, la esquizofrenia o las neurodegeneraciones son debidas en buena medida a fallos o malfuncionamientos de nuestras redes biológicas. Los conflictos sociales, e incluso las guerras, dependen en gran medida de las estructuras de las redes que se forman entre los individuos, grupos y países. Sin embargo, este libro nos enseña que las redes están también en las soluciones de todos estos y de otros muchos problemas. ¿Es cierto entonces que estamos a merced de las redes? A merced de las redes te hará más libre para responder a esta y a otras preguntas acuciantes de nuestro mundo actual porque «Sólo el que sabe es libre y es más libre quien más sabe» y este libro te hará más sabio y por tanto más libre.

A MERCED
DE LAS REDES

ERNESTO ESTRADA ROGER

A MERCED DE LAS REDES



ERNESTO ESTRADA ROGER

Ernesto Estrada Roger es profesor de investigación (catedrático) del Consejo Superior de Investigaciones Científicas (CSIC) en el Instituto de Física Interdisciplinar y Sistemas Complejos (IFISC) de Palma de Mallorca. Ha publicado más de 200 trabajos científicos y dos libros de texto (en inglés) en las áreas de estudio de los sistemas complejos.

Es miembro honorífico de la Sociedad de Matemáticas Industrial y Aplicadas (SIAM), de la Academia Europea, de la Academia de Ciencias de Latinoamérica (ACAL) y del Instituto de Matemáticas y sus Aplicaciones (IMA) del Reino Unido. Por sus trabajos ha recibido varias distinciones como el Premio Wolfson al Mérito Científico de la Real Sociedad de Londres en Reino Unido y ha sido conferenciante plenario en diversos eventos científicos de matemática aplicada, tales como la conferencia anual de SIAM en 2012 o el XXVI Congreso bial de la Sociedad Española de Matemática Aplicada (SeMA) en 2020. Ha desarrollado labores divulgativas en varios medios de prensa (ABC, El País), así como en escuelas de verano y congresos internacionales. Actualmente reside en Valldemossa, Islas Baleares.

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**Thank
you!**

How bypasses affect dynamics on networks?

Synchronization

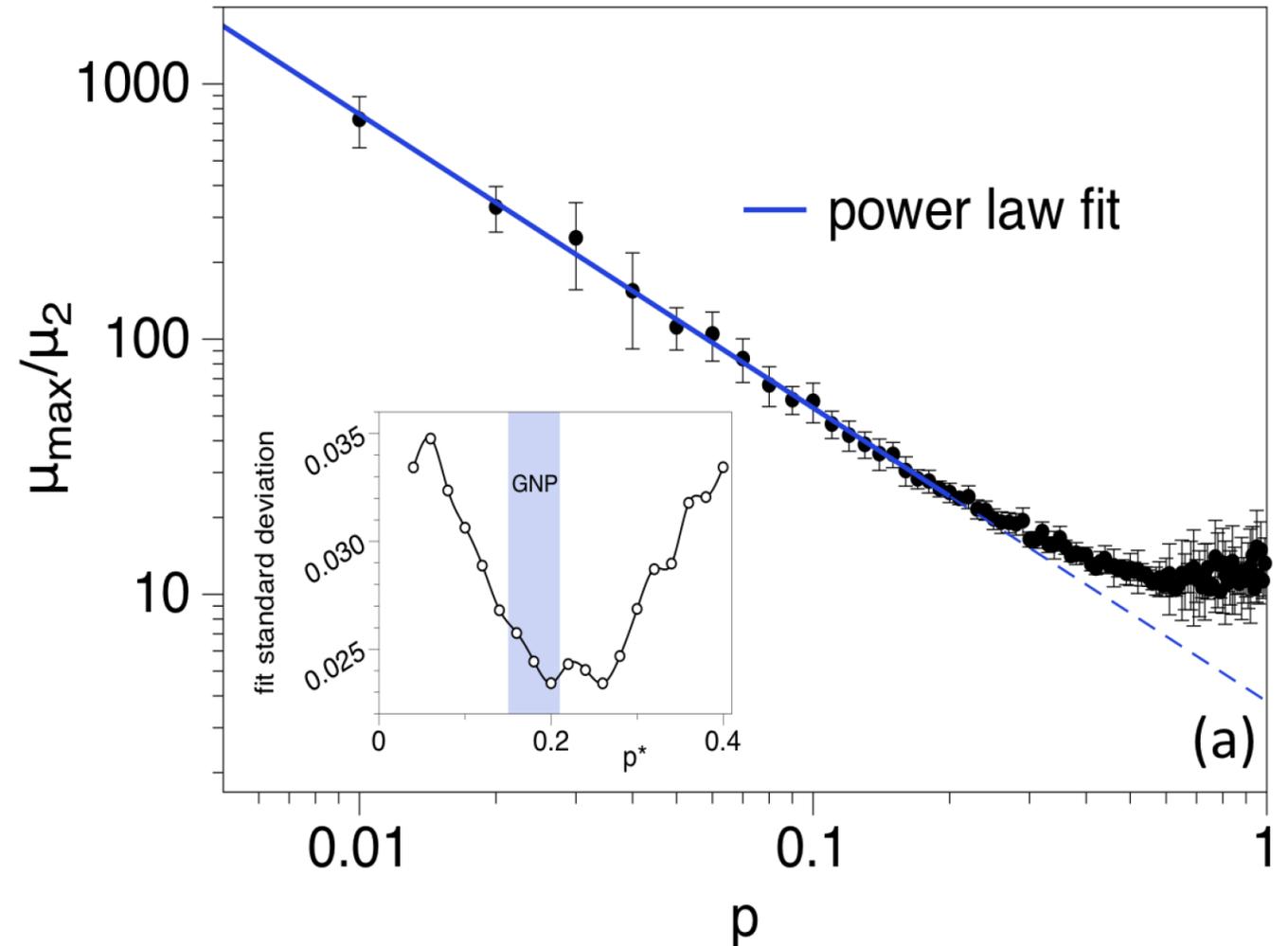
$$\dot{x}_i = F(x_i) - \sigma \sum_{j=1}^n L_{ij} H(x_j)$$

Synchronizability

Let $0 = \mu_1 < \mu_2 \leq \dots \leq \mu_{\max}$ be the eigenvalues of L . Network synchronizability is quantified by the ratio

$$Q := \frac{\mu_{\max}}{\mu_2},$$

such that the smaller the eigenratio Q , the easier it is to synchronize the oscillators.



How bypasses affect dynamics on networks?

Epidemic spreading

Epidemic threshold

Let β be the infection rate and δ be the curing rate for a disease spreading according to the model:

$$\dot{p}_i(t) = \beta \left(1 - p_i(t)\right) \sum_{j \in \eta_i} A_{ij} p_j(t) - \delta p_i(t)$$

Then, infection will die out exponentially if the infection strength $\tau := \beta / \delta$ satisfies:

$$\tau \leq \frac{1}{\lambda_1(A)}.$$

