

Machine intelligence and network science for complex systems big data analysis



Carlo Vittorio Cannistraci

Center for Complex Network Intelligence (CCNI)

Tsinghua Laboratory of Brain and Intelligence



清华大学
Tsinghua University



清华大学脑与智能实验室
Tsinghua Laboratory of Brain and Intelligence

OUTLINE of the talk

1. Prediction of connectivity in sparse network structures
2. Dynamic sparse training in deep learning
3. Neuromorphic computing



Carlo V. Cannistraci Prof. PhD. Eng.

Zhou Yahui Chair Professor

Chief Scientist, Tsinghua Laboratory of Brain and Intelligence (THBI)

Director, Center for Complex Network Intelligence (CCNI) at THBI

If physics studies the principles and mechanisms of the outside universe.

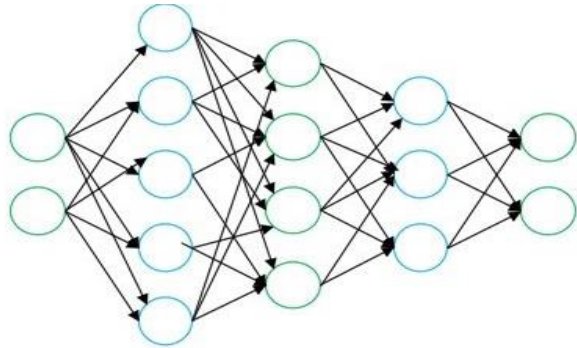
Brain science studies the principles and mechanisms of the inside universe.

My research is at the interface between these two disciplines.

I deal with "Physics and Engineering of Complexity and Intelligence": studying principles of natural and artificial intelligence.

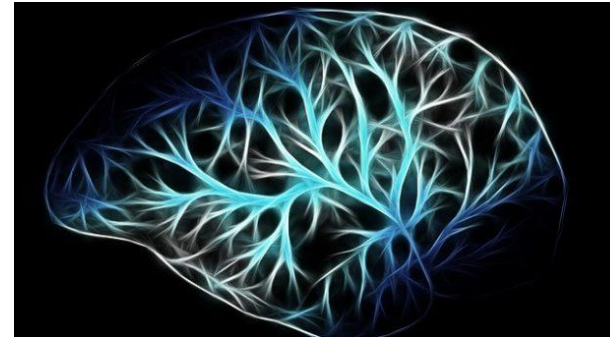
Crisis: I was a Master student in 2002

Artificial Neural Network (ANN)



Vs.

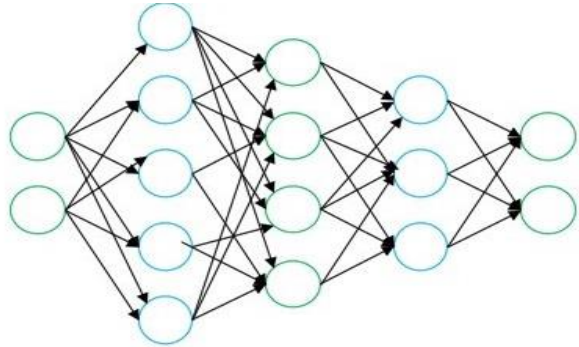
Brain Connectivity



Crisis: Why is brain connectivity sparse?

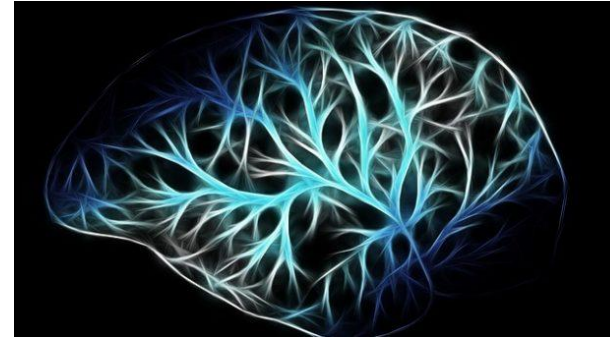
Crisis: I was a Master student in 2002

Artificial Neural Network (ANN)



Vs.

Brain Connectivity

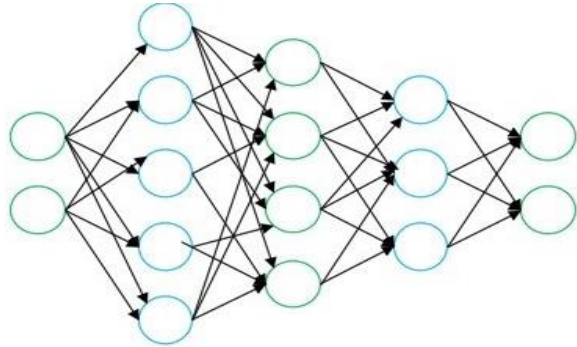


Crisis: Why is brain connectivity sparse?

- 1. What is the computational advantage of connectivity sparsity in brain biology?***

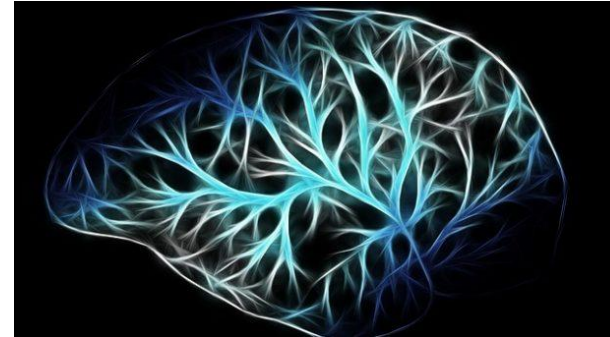
Crisis: I was a Master student in 2002

Artificial Neural Network (ANN)



Vs.

Brain Connectivity

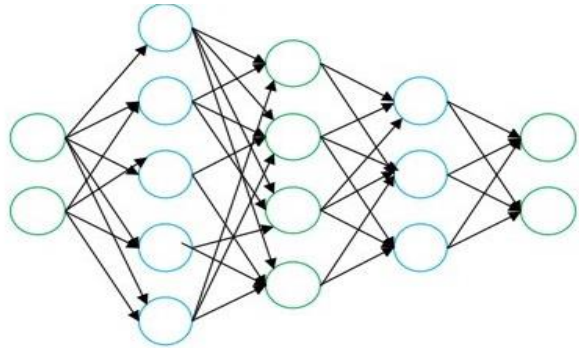


Crisis: Why is brain connectivity sparse?

- 1. What is the computational advantage of connectivity sparsity in brain biology?*
- 2. How to make profit of brain-inspired connectivity sparsity in ANN?*

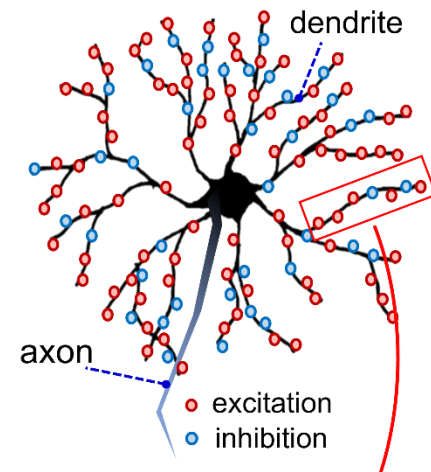
Crisis: I was a Master student in 2002

Artificial Neural Network (ANN)



Vs.

Brain Morphology

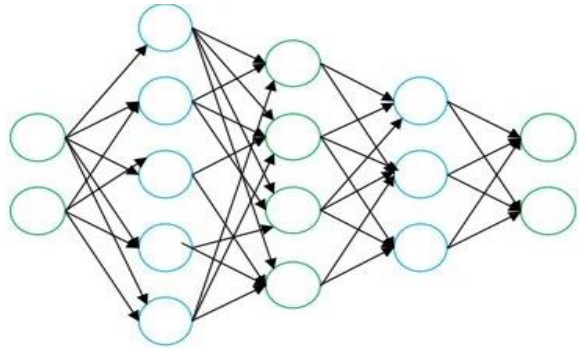


Crisis: Why is brain connectivity sparse (**topology**)?

Crisis: What is the contribution of **morphology**?

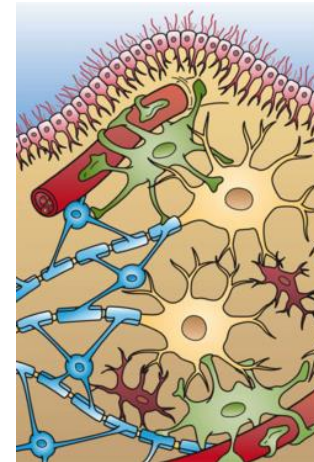
Crisis: I was a Master student in 2002

Artificial Neural Network (ANN)



Vs.

Brain cell coupling



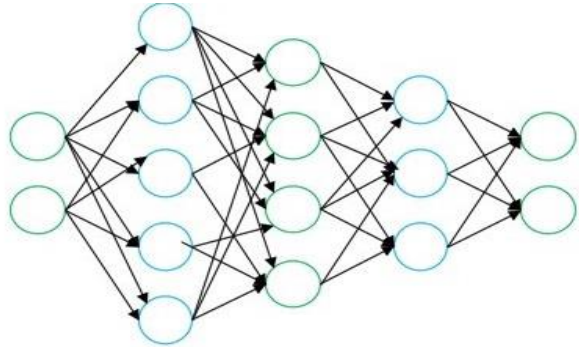
Crisis: Why is brain connectivity sparse (**topology**)?

Crisis: What is the contribution of **morphology**?

Crisis: What is the contribution of **neuro-glia coupling**?

Crisis: I was a Master student in 2002

Artificial Neural Network (ANN)



Vs.

Brain Connectivity



Crisis: Why is brain connectivity sparse (**topology**)?

Crisis: What is the contribution of morphology?

Crisis: What is the contribution of neuro-glia coupling?

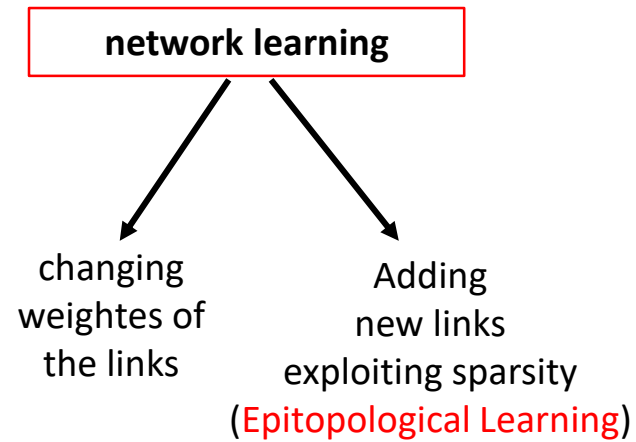
My master student 'Obsession'!
(2002)



Donald Olding Hebb
(July 22, 1904 – August 20, 1985)
psychologist

He is best known for his theory of **Hebbian learning**, which he introduced in his classic 1949 work ***The Organization of Behavior***. He has been described as the father of neuropsychology and **neural networks**.

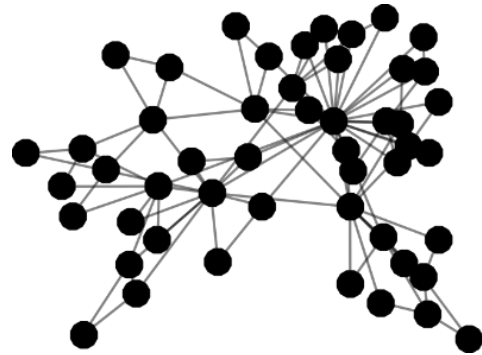
neurons that fire together wire together



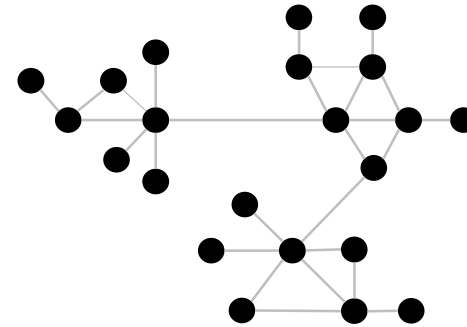
Complex network intelligence

Connectivity \leftrightarrow Function

How network connectivity influence function in complex systems, in particular learning and intelligence. But also the reverse.

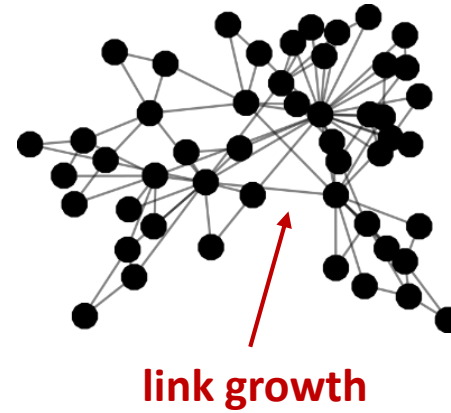


Shape 1

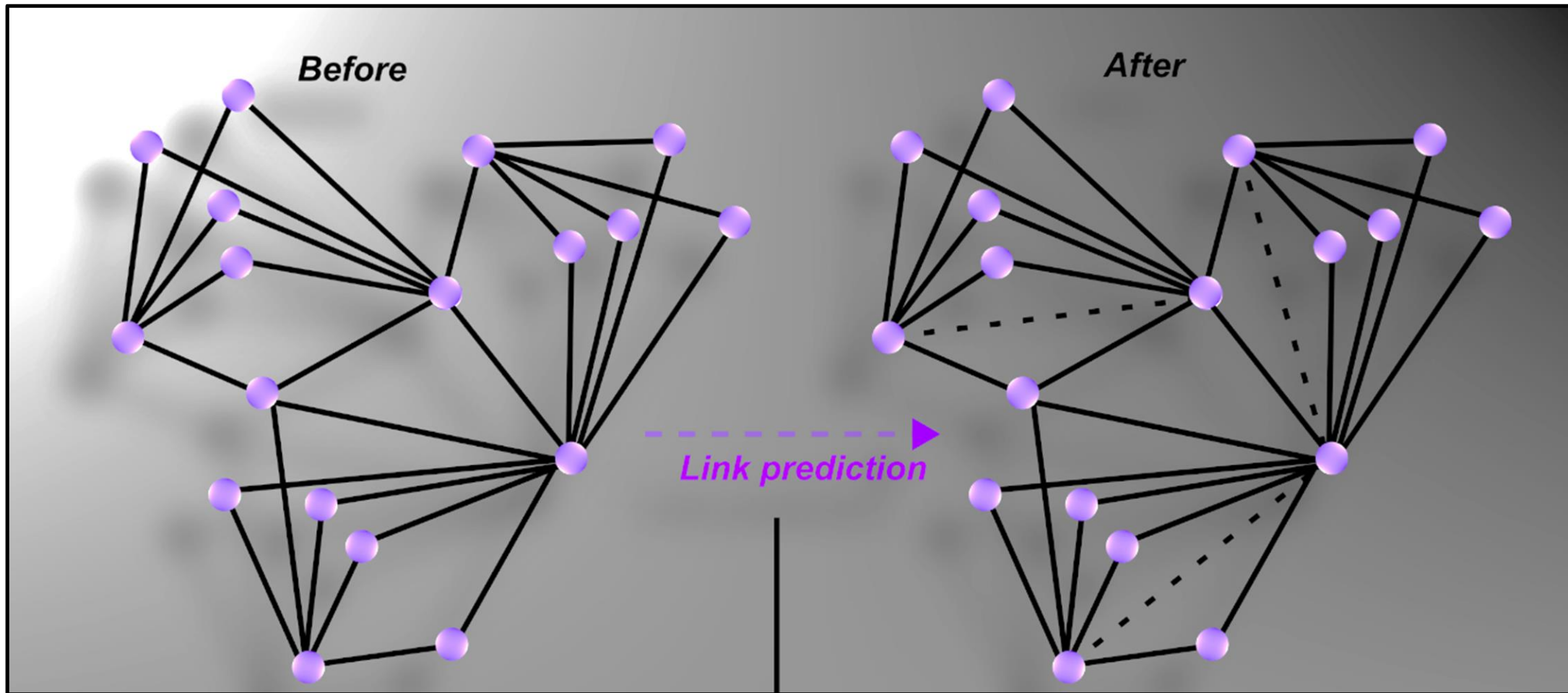


Shape 2

NETWORK TOPOLOGY MODELS AND MECHANISMS



How to model link connectivity in complex networks?





Apr 2013



SUBJECT AREAS:
NETWORK TOPOLOGY
NETWORK MODELS
COMPLEX NETWORKS
COMPLEXITY

From link-prediction in brain connectomes and protein interactomes to the local-community-paradigm in complex networks

Carlo Vittorio Cannistraci^{1,2*}, Gregorio Alanis-Lobato^{1,2*} & Timothy Ravasi^{1,2}

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Correspondence and requests for materials should be addressed to C.V.C. (kalokagathos.agon@gmail.com) or T.R. (timothy.ravasi@kaust.edu.sa)

¹Integrative Systems Biology Laboratory, Biological and Environmental Sciences and Engineering Division, Computer, Electrical and Mathematical Sciences and Engineering Division, Computational Bioscience Research Center, King Abdullah University of Science and Technology (KAUST), Ibn Al Haytham Bldg. 2, Level 4, Thuwal 23955-6900, Kingdom of Saudi Arabia, ²Division of Medical Genetics, Department of Medicine, University of California, San Diego, 9500 Gilman Drive, La Jolla, CA 92093 USA.

Growth and remodelling impact the network topology of complex systems, yet a general theory explaining how new links arise between existing nodes has been lacking, and little is known about the topological properties that facilitate link-prediction. Here we investigate the extent to which the connectivity evolution of a network might be predicted by mere topological features. We show how a link/community-based strategy triggers substantial prediction improvements because it accounts for the singular topology of several real networks organised in multiple local communities - a tendency here named *local-community-paradigm* (LCP). We observe that LCP networks are mainly formed by weak interactions and characterise heterogeneous and dynamic systems that use self-organisation as a major adaptation strategy. These systems seem designed for global delivery of information and processing via multiple local modules. Conversely, non-LCP networks have steady architectures formed by strong interactions, and seem designed for systems in which information/energy storage is crucial.

- From link-prediction in brain connectomes and protein interactomes to the local-community-paradigm in complex networks

CV Cannistraci, G Alanis-Lobato, T Ravasi
Scientific reports 3 (1), 1-14

408

2013

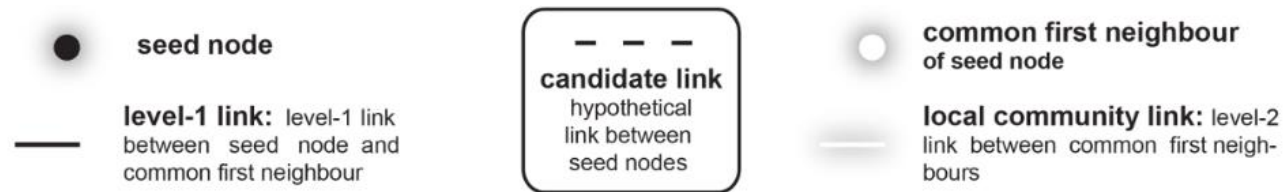
Local Community Paradigm (LCP)

Explicative example: how CAR-Index predicts the likelihood of candidate links

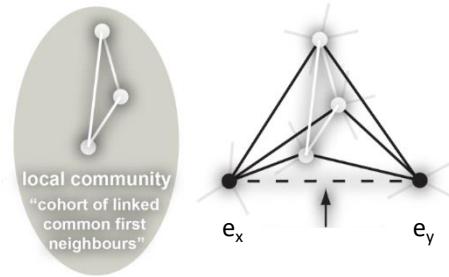


CN-Index = # common first neighbours

CAR-Index = (# common first neighbours) x (# local community links)

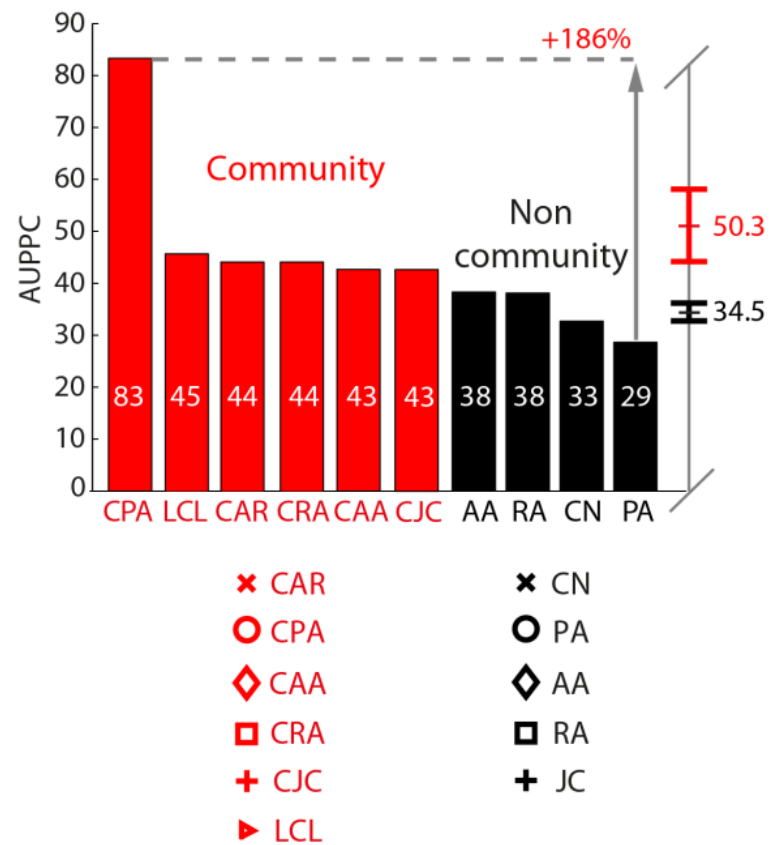
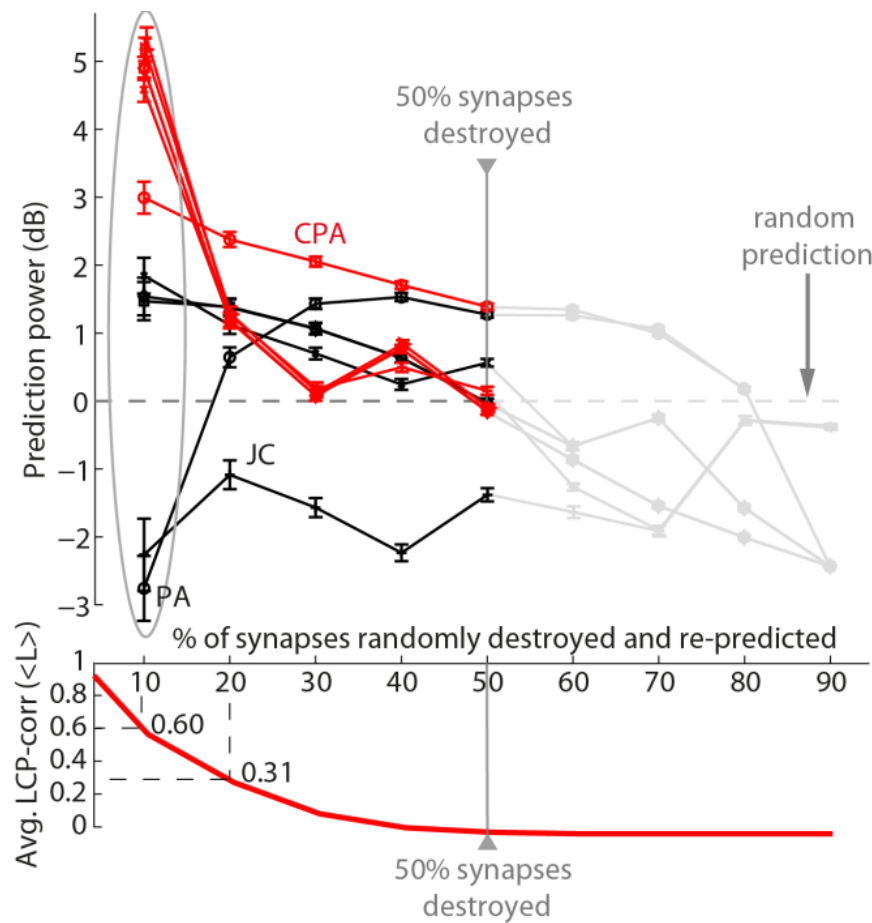


The LCP-trick:
how to covert
classical neighbourhood
indices in
local-community indices

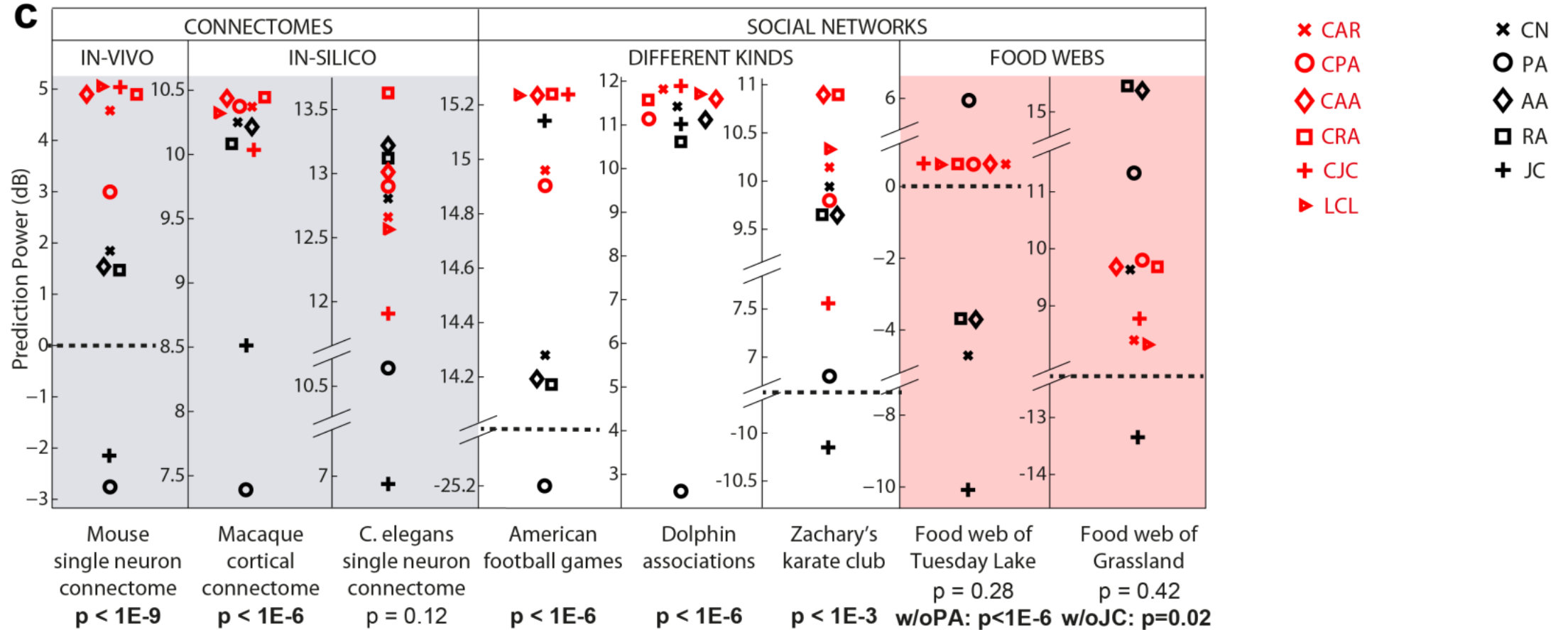


Type	Name of the Index	Formulation
Classical	Common Neighbours (CN)	$CN(x, y) = \Gamma(x) \cap \Gamma(y) = i_x = i_y$
	Preferential Attachment (PA)	$PA(x, y) = \Gamma(x) \cdot \Gamma(y) = (e_x + i_x) \cdot (e_y + i_y) = e_x e_y + e_x CN(x, y) + e_y CN(x, y) + CN(x, y)^2$
	Adamic & Adar (AA)	$AA(x, y) = \sum_{s \in \Gamma(x) \cap \Gamma(y)} \frac{1}{\log_2(\Gamma(s))}$
	Resource Allocation (RA)	$RA(x, y) = \sum_{s \in \Gamma(x) \cap \Gamma(y)} \frac{1}{ \Gamma(s) }$
	Jaccard (JC)	$JC(x, y) = \frac{ \Gamma(x) \cap \Gamma(y) }{ \Gamma(x) \cup \Gamma(y) } = \frac{CN(x, y)}{ \Gamma(x) \cup \Gamma(y) }$
LCP-based	CAR	$CAR(x, y) = CN(x, y) \cdot LCL(x, y) = CN(x, y) \cdot \sum_{s \in \Gamma(x) \cap \Gamma(y)} \frac{ \gamma(s) }{2}$
	CPA	$CPA(x, y) = e_x e_y + e_x CAR(x, y) + e_y CAR(x, y) + CAR(x, y)^2$
	CAA	$CAA(x, y) = \sum_{s \in \Gamma(x) \cap \Gamma(y)} \frac{ \gamma(s) }{\log_2(\Gamma(s))}$
	CRA	$CRA(x, y) = \sum_{s \in \Gamma(x) \cap \Gamma(y)} \frac{ \gamma(s) }{ \Gamma(s) }$
	CJC	$CJC(x, y) = \frac{CAR(x, y)}{ \Gamma(x) \cup \Gamma(y) }$

LINK PREDICTION IN BRAIN CONNECTOMES AND MORE



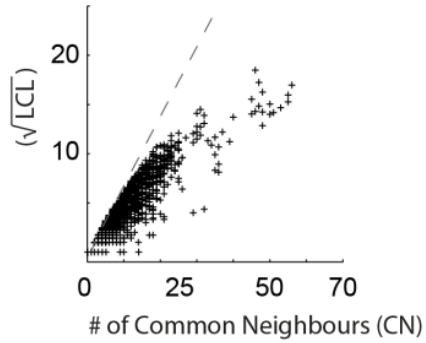
LINK PREDICTION IN BRAIN CONNECTOMES AND MORE



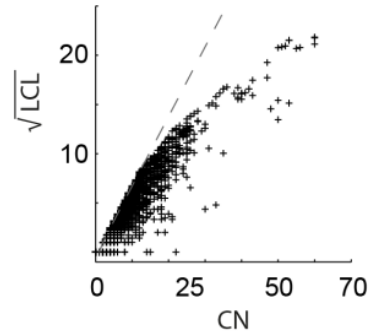
What is behind this performance in network connectivity prediction?

LOCAL COMMUNITY PARADIGM (LCP) IN REAL NETWORKS

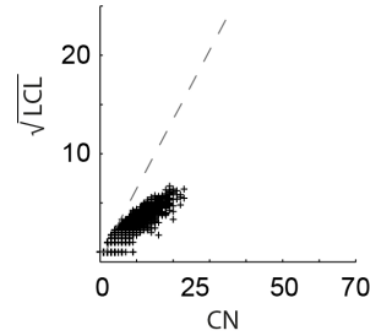
Network1 (Ben-Hur et al., 2005)
Nodes = 4036, Links = 10411



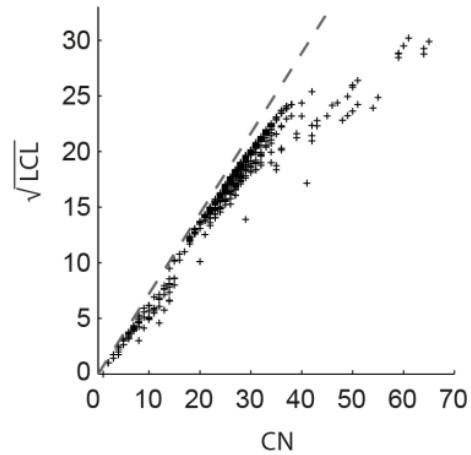
Network2 (Chen et al., 2006)
Nodes = 4385, Links = 12234



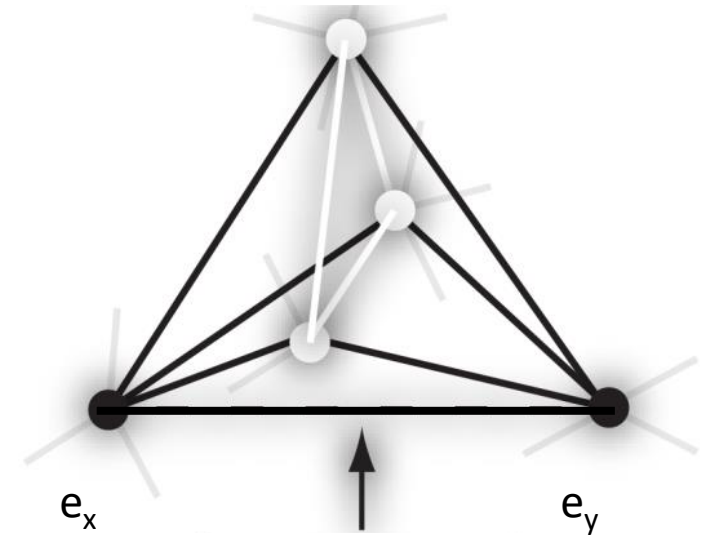
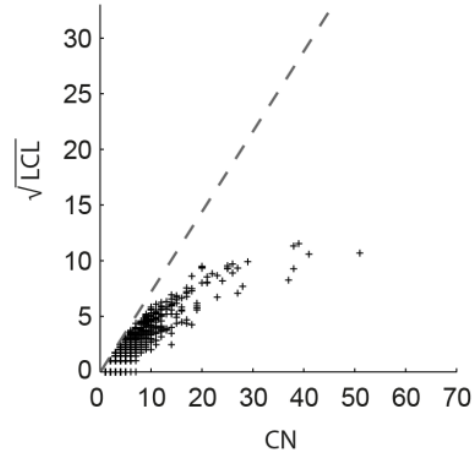
Network3 (You et al., 2010)
Nodes = 3645, Links = 12934



Macaque Cortical Connectome
Nodes = 94, Links = 1515

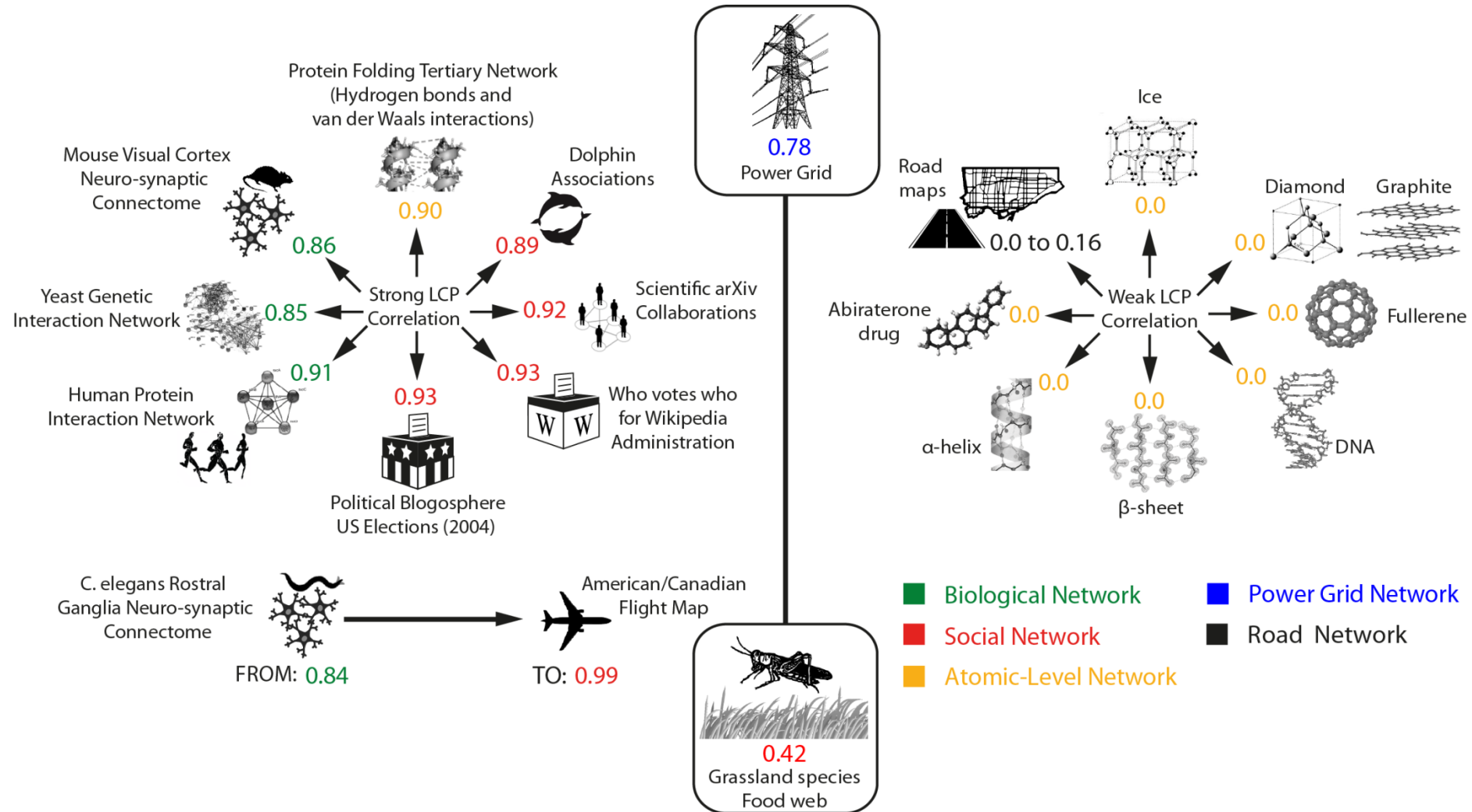


C. elegans Rostral Ganglia Neuro-synaptic Connectome
Nodes = 131, Links = 687



$$LCP_{corr} = \frac{\text{cov}(CN, LCL)}{\sigma_{CN} \cdot \sigma_{LCL}}, \text{ when } CN > 0$$

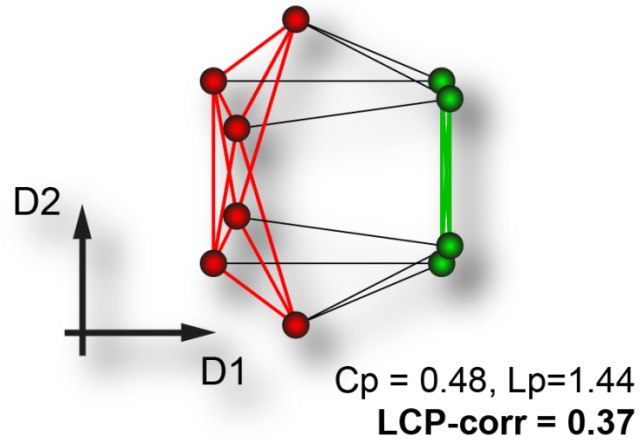
**The LCP points out a dichotomy
between
the structure of many real networks
(see figure below)**



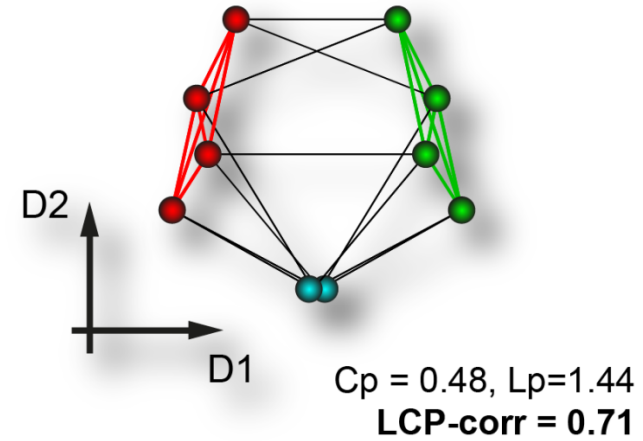
LOCAL COMMUNITY PARADIGM IN IDEALISED NETWORKS

a

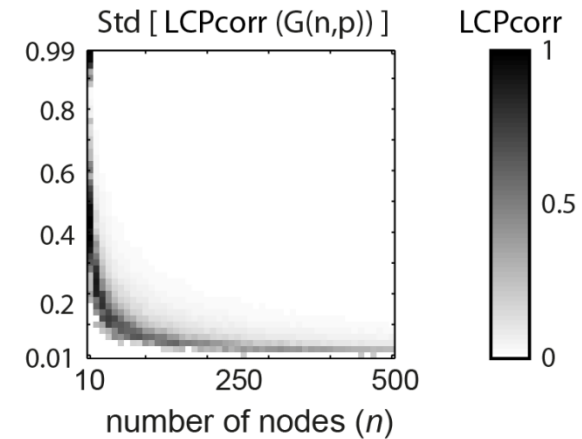
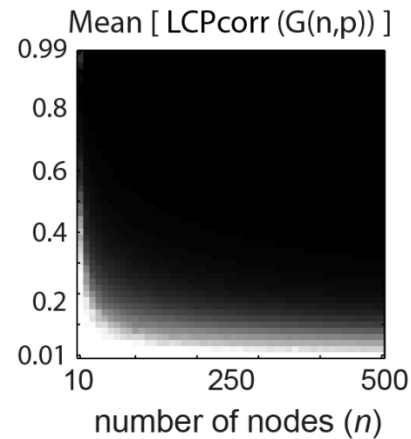
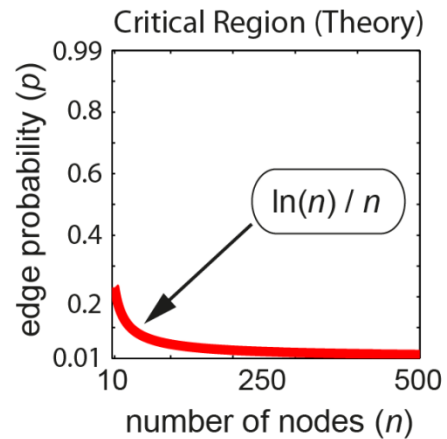
Isomap reveals the presence
of two clusters discriminated by D1



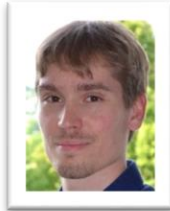
Isomap reveals the presence
of three clusters discriminated by D1



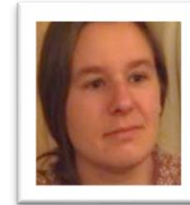
b



Simone



Phine



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with: Deutsche Physikalische
Gesellschaft and the Institute
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PAPER

Common neighbours and the local-community-paradigm for topological link prediction in bipartite networks

Simone Daminelli^{1,4}, Josephine Maria Thomas^{2,4}, Claudio Durán^{2,3} and Carlo Vittorio Cannistraci²

¹ Bioinformatics Group, Biotechnology Center (BIOTEC), Technische Universität Dresden, Dresden, Germany

² Biomedical Cybernetics Group, Biotechnology Center (BIOTEC), Technische Universität Dresden, Dresden, Germany

³ Escuela de Ingeniería en Bioinformática, Universidad de Talca, 2 Norte #685, 3465548, Talca, Chile

⁴ These authors contributed equally to this work.

E-mail: kalokagathos.agon@gmail.com

Keywords: complex systems and networks, interdisciplinary physics, biological physics, link prediction, bipartite networks, networks models

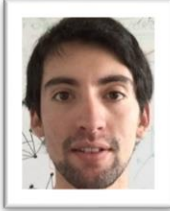
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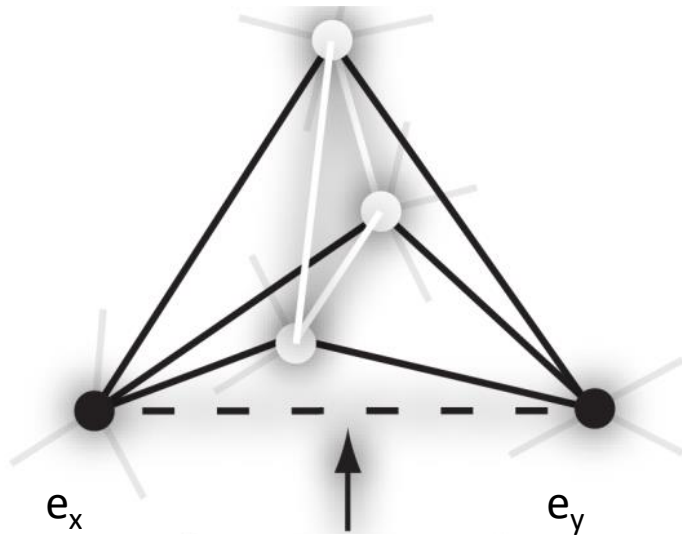
Claudio



Abstract

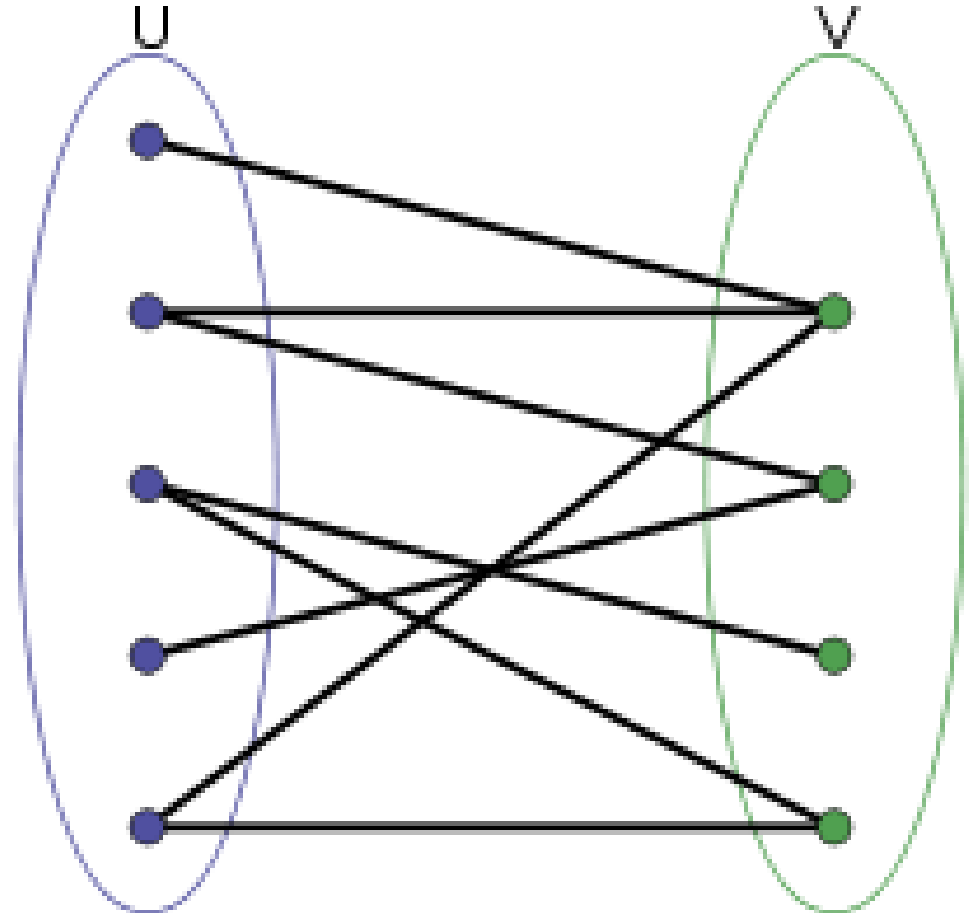
Bipartite networks are powerful descriptions of complex systems characterized by two different classes of nodes and connections allowed only across but not within the two classes. Unveiling physical principles, building theories and suggesting physical models to predict bipartite links such as product-consumer connections in recommendation systems or drug-target interactions in molecular networks can provide priceless information to improve e-commerce or to accelerate pharmaceutical research. The prediction of complex network connections starting from the knowledge present in the

Monopartite graph



Triadic closure

Bipartite graph



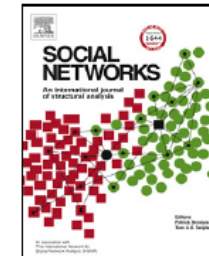
~~Triadic closure~~



Contents lists available at ScienceDirect

Social Networks

journal homepage: www.elsevier.com/locate/socnet



Triadic closure in two-mode networks: Redefining the global and local clustering coefficients

Tore Opsahl*

Imperial College Business School, Imperial College London, London, United Kingdom

ARTICLE INFO

Keywords:

Clustering coefficient
Random networks
Triadic closure
Two-mode networks

ABSTRACT

As the vast majority of network measures are defined for one-mode networks, two-mode networks often have to be projected onto one-mode networks to be analyzed. A number of issues arise in this transformation process, especially when analyzing ties among nodes' contacts. For example, the values attained by the global and local clustering coefficients on projected random two-mode networks deviate from the expected values in corresponding classical one-mode networks. Moreover, both the local clustering coefficient and constraint (structural holes) are inversely associated to nodes' two-mode degree. To overcome these issues, this paper proposes redefinitions of the clustering coefficients for two-mode networks.

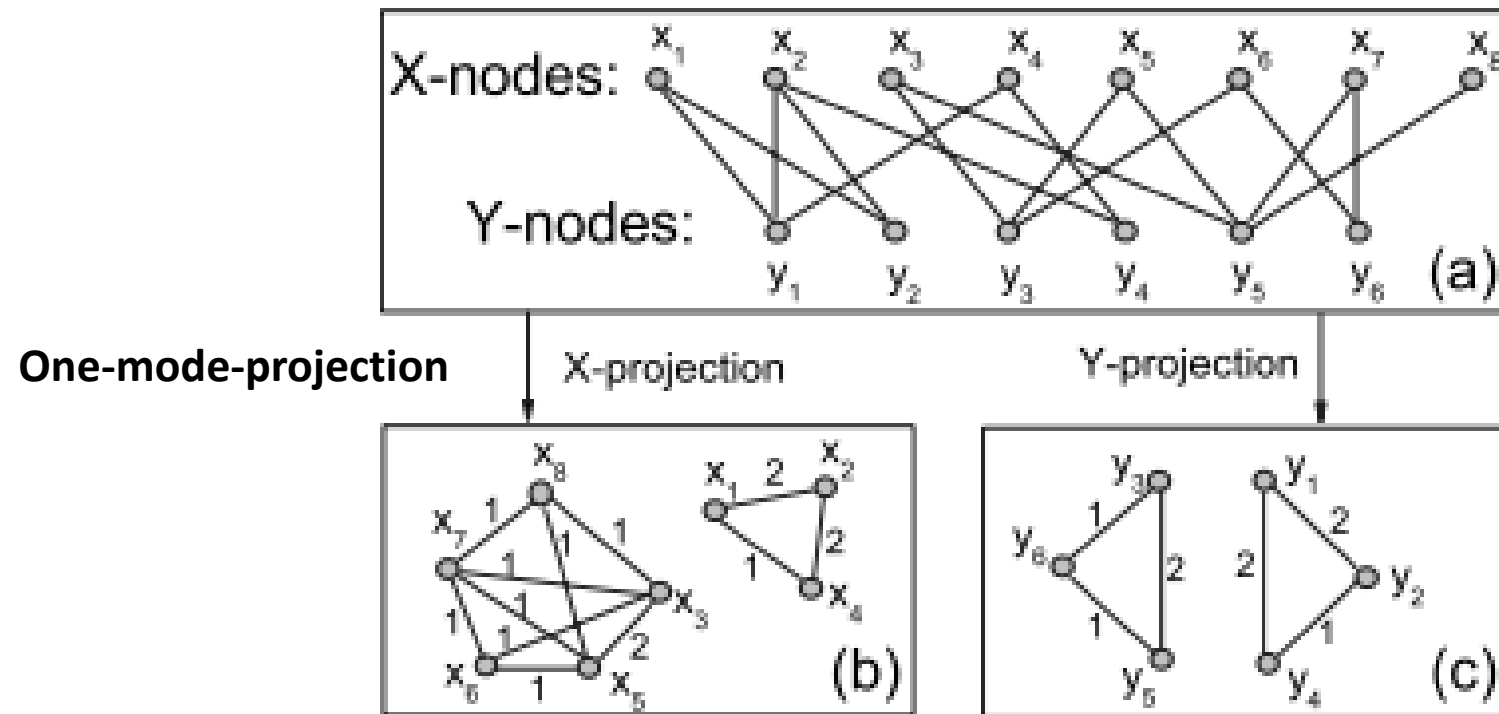
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Zhou, T. et al., **2007**. Bipartite network projection and personal recommendation.
Phys Rev E Stat Nonlin Soft Matter Phys, 76(4 Pt 2), p.46115.

Network based inference (NBI, also known as Probs) (tuning-free)

Zhou, T. et al., **2010**. Solving the apparent diversity- accuracy dilemma of recommender systems.
Proceedings of the National Academy of Sciences of the United States of America, 107(10), pp.4511–5.

HeatS + Probs (one parameter to tune)



Using Random Walks to Generate Associations between Objects

Bipartite projection via random-walk (BPR)

Muhammed A. Yildirim*, Michele Coscia

Center for International Development, Harvard University, Cambridge, Massachusetts, United States of America

Abstract

Measuring similarities between objects based on their attributes has been an important problem in many disciplines. Object-attribute associations can be depicted as links on a bipartite graph. A similarity measure can be thought as a unipartite projection of this bipartite graph. The most widely used bipartite projection techniques make assumptions that are not often fulfilled in real life systems, or have the focus on the bipartite connections more than on the unipartite connections. Here, we define a new similarity measure that utilizes a practical procedure to extract unipartite graphs without making *a priori* assumptions about underlying distributions. Our similarity measure captures the relatedness between two objects via the likelihood of a random walker passing through these nodes sequentially on the bipartite graph. An important aspect of the method is that it is robust to heterogeneous bipartite structures and it controls for the transitivity similarity, avoiding the creation of unrealistic homogeneous degree distributions in the resulting unipartite graphs. We test this method using real world examples and compare the obtained results with alternative similarity measures, by validating the actual and orthogonal relations between the entities.

Citation: Yildirim MA, Coscia M (2014) Using Random Walks to Generate Associations between Objects. PLoS ONE 9(8): e104813. doi:10.1371/journal.pone.0104813

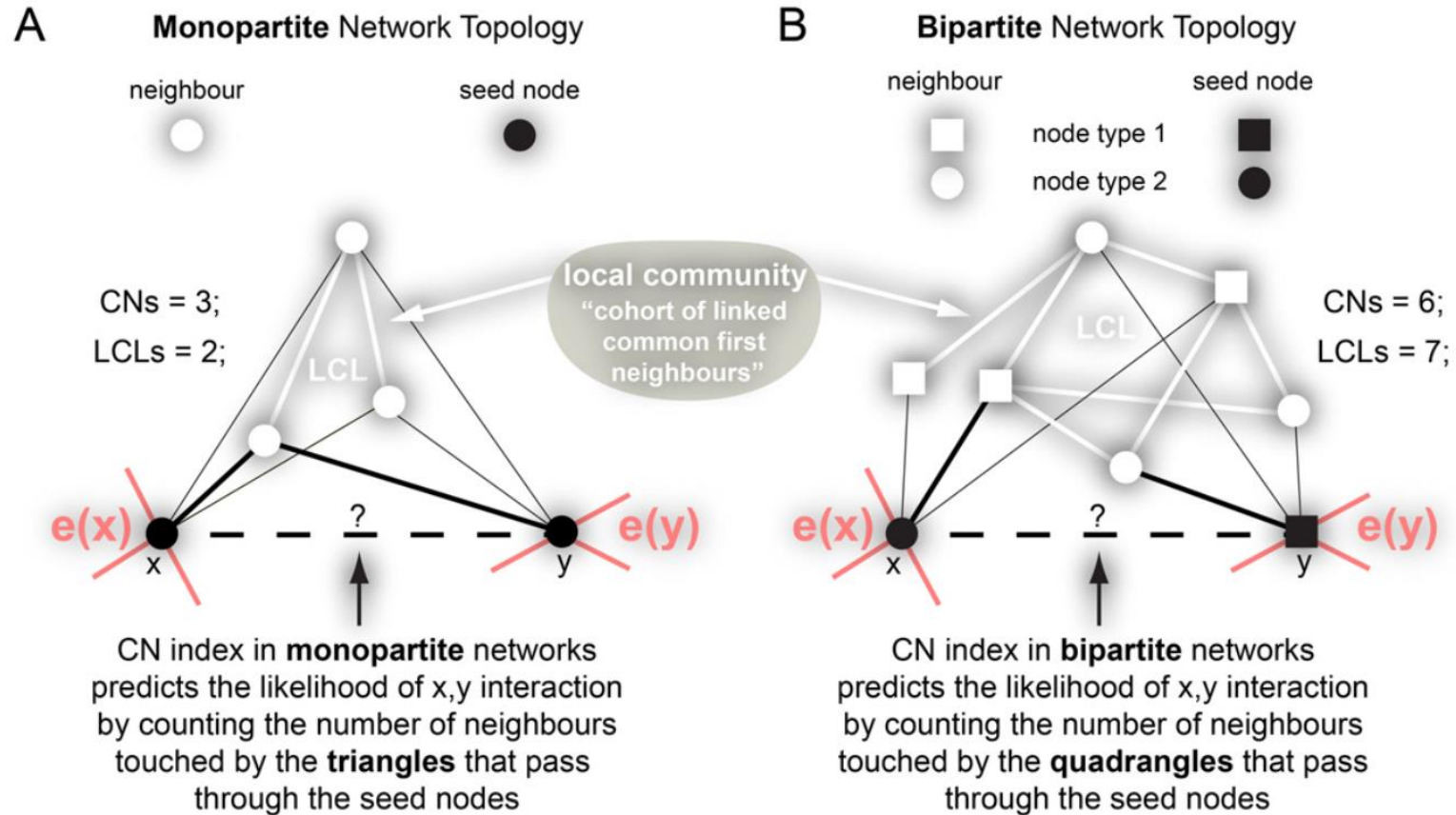
Editor: Fabio Rapallo, University of East Piedmont, Italy

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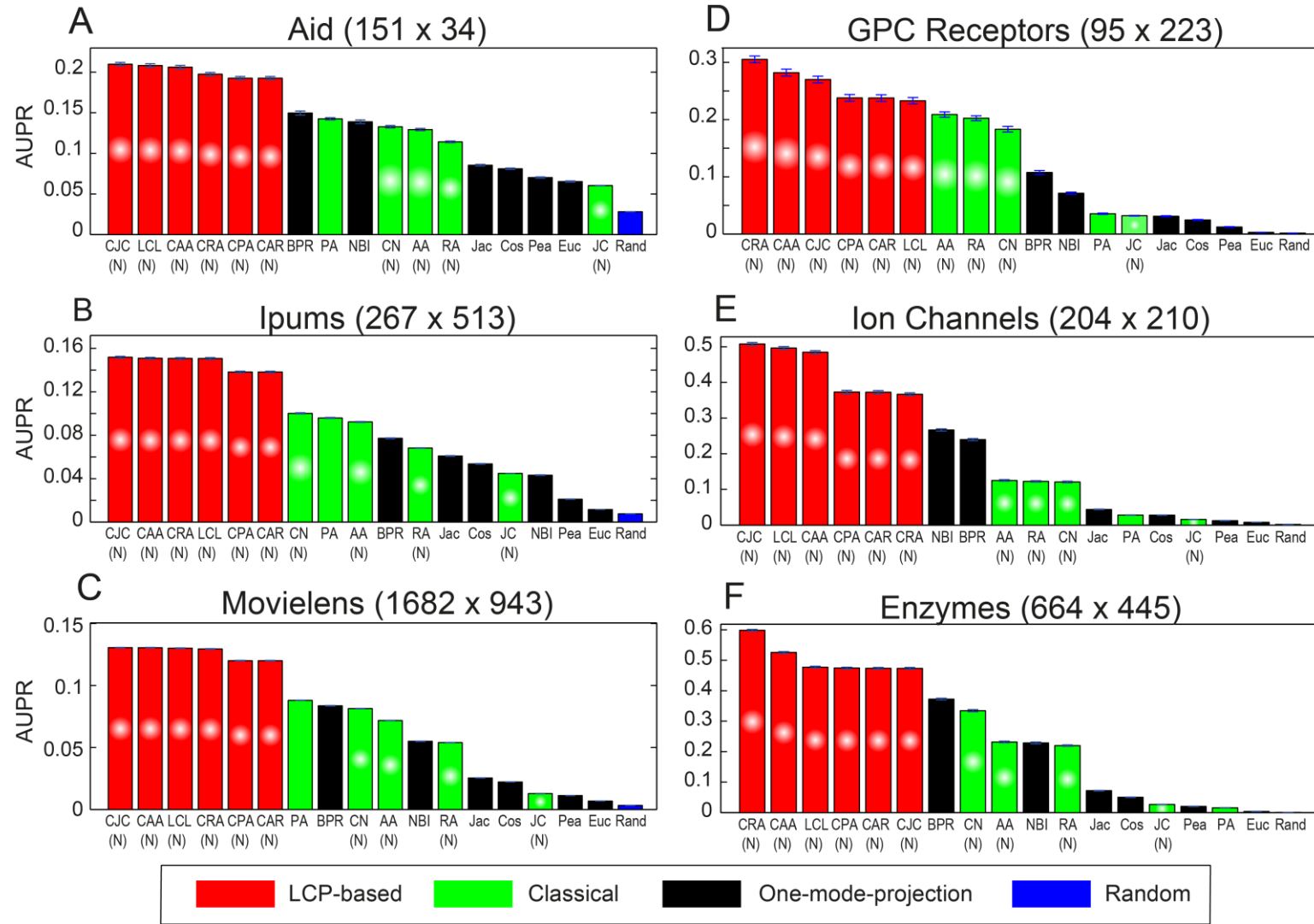
Data Availability: The authors confirm that all data underlying the findings are fully available without restriction. All relevant data are within the paper and its Supporting Information files.

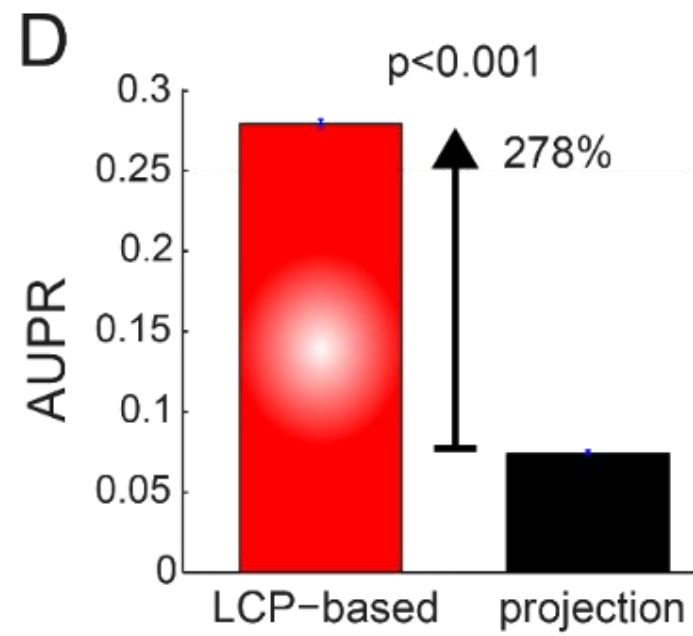
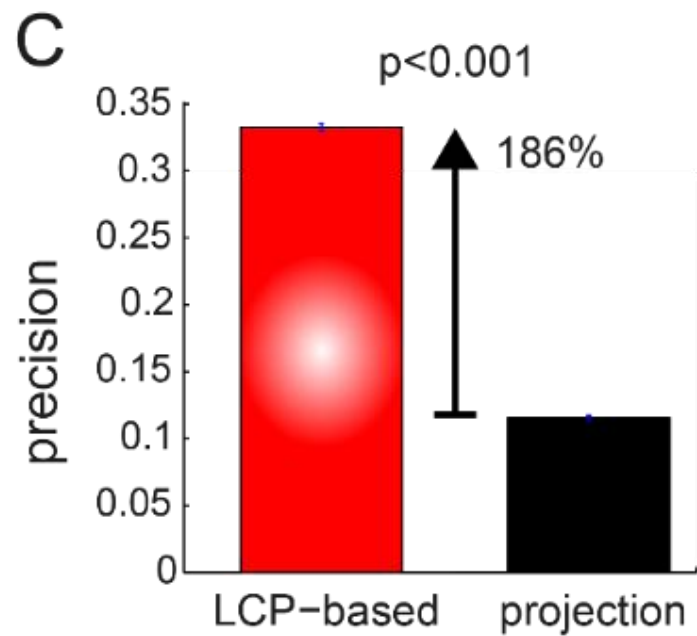
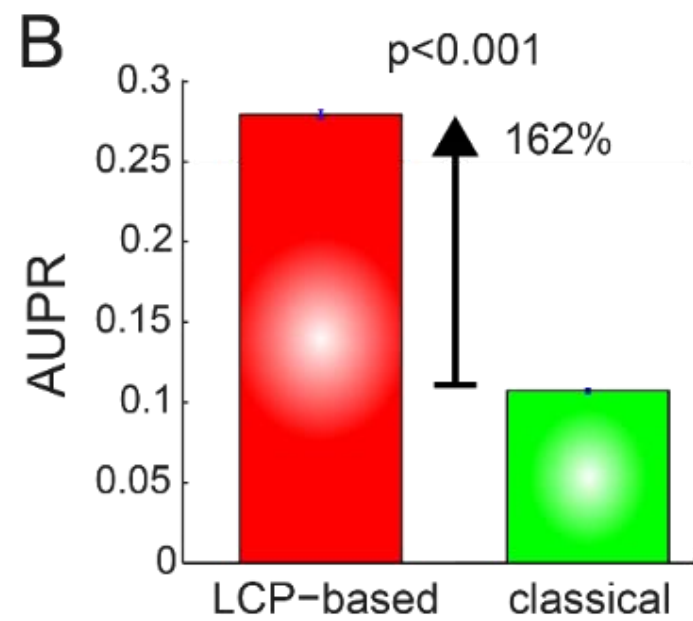
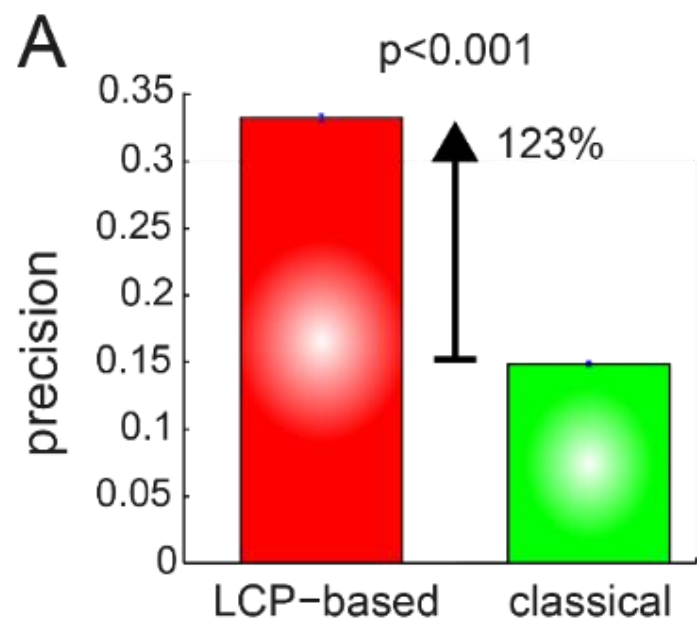
From monopartite to bipartite



From triangles to quadrangles: From L2 to L3

Daminelli, ... and Cannistraci Common neighbours and the local-community-paradigm for topological link prediction in bipartite networks. **New J. Phys. (2015).**





**CD-Based Indices
for
Link Prediction in
Complex Network**
Tao Wang et al.
Plos One 2016

	1	2	3	4	5	6	7	Mean
	USAir	Neural	Word	PB	Jazz	Email	FT	
	(-0.208)	(-0.1632)	(-0.1293)	(-0.079)	(0.0202)	(0.0782)	(0.1624)	
CN	82.26059	20.2745	11.44615	70.56	31.44099	77.58659	28.37255	45.99163
Salton	11.8002	5.0095	0	3.96	33.56522	24.024	34.15686	16.07368
PA	70.5669	12.4485	15.73846	26.84	8.10559	9.445799	0.029412	20.45352
Sorensen	15.8046	6.192	0	7.84	32.83851	35.3808	33.84314	18.84272
LHN	2.1939	0	0	0.2	6.322981	0.9828	38.26471	6.852055
RA	100.3656	21.371	9.446154	62.48	33.52174	79.00619	27.70588	47.69951
LP3	81.40859	21.3495	12.49231	73.12	29.36025	74.69279	25.79412	45.45965
LP4	79.40639	20.597	16.46154	72.84	27.82609	72.61799	26.56863	45.18823
LRW	25.3683	30.4225	10.30769	38	22.1677	36.4182	24.81373	26.78544
LB	78.65957	18.34043	15.67692	58.48	17.09938	47.33333	18.28431	36.2677
CAR	80.32229	19.8015	8.446154	69.16	32.21739	76.54919	33	45.64236
CPA	80.47139	21.07	10.69231	69.2	32.09938	70.59779	32.57843	45.24419
CAA	80.76959	21.5215	7.230769	69.24	33.15528	78.29639	35.05882	46.46748
CRA	85.79639	24.725	7.553846	71.84	34.73292	85.55819	35.10784	49.3306
CJC	76.40309	15.0715	3.830769	64.64	34.58385	83.15579	34.93137	44.65948
CD-LD	81.81329	21.0055	4.584615	70.6	31.85093	80.69879	30.5	45.86473
CD-LD-2	88.99139	17.9955	16.30769	70.32	32.07453	75.40259	33.20588	47.7568
CD-LD-3	88.99139	17.9955	15.73846	70.56	32.52174	73.38239	34.78431	47.71054
CD-LD-4	88.99139	21.0055	15.07692	70.32	32.52174	76.98599	34	48.41451
CD-LD-5	88.99139	21.0055	15.03077	70.2	32.52174	79.00619	34	48.67937
CD-LD-6	88.99139	21.0055	15.03077	70.2	32.52174	79.60679	34	48.76517
CD*LD	81.77069	19.6725	6.076923	70.72	32.21118	79.98899	31.29412	45.96206
CD*LD-2	87.99029	17.501	6.876923	70.2	32.52174	73.21859	32.41176	45.81719
CD*LD-3	88.99139	15.996	11.16923	70.68	33.19876	73.00019	35.57843	46.94486
CD*LD-4	88.99139	17.9955	11.16923	70.56	33.19876	76.98599	35.57843	47.78276
CD*LD-5	88.99139	17.9955	11.16923	70.56	33.19876	78.78779	35.57843	48.04016
CD*LD-6	88.99139	17.9955	12.01538	70.68	33.19876	79.38839	35.57843	48.26398
CD	1.8105	1.0965	0.892308	0.4	16.08075	6.551999	34.08824	8.702898
CD-2	4.0044	1.9995	1.2	1.2	22.36025	16.8168	23.71569	10.18523
CD-3	4.0044	1.0105	1.2	0.6	22.36025	26.4264	36.37255	13.13916
CD-4	3.0033	1.0105	1.2	0.48	18.97516	17.4174	37.15686	11.32046
CD-5	3.0033	1.0105	1.2	0.72	18.29193	6.388199	37.15686	9.681541
CD-6	3.0033	1.0105	1.2	0.72	18.29193	5.4054	37.15686	9.541141
CDI	71.3976	11.997	11.44615	29.04	8.720497	14.0322	0.313725	20.99245






2019

ARTICLE

<https://doi.org/10.1038/s41467-019-09177-y>

OPEN

Network-based prediction of protein interactions

István A. Kovács^{1,2,3}, Katja Luck ^{2,4}, Kerstin Spirohn^{2,4}, Yang Wang^{2,4}, Carl Pollis ^{2,4}, Sadie Schlabach^{2,4},
Wenting Bian^{2,4}, Dae-Kyum Kim^{2,5}, Nishka Kishore^{2,5}, Tong Hao^{2,4}, Michael A. Calderwood ^{2,4},
Marc Vidal^{2,4} & Albert-László Barabási^{1,2,6,7}

**[...] the best performing literature method, Cannistraci Resource Allocation (CRA),
out of 23 different methods tested.**

Why is CRA so powerful in link prediction?

Understanding link prediction via geometrical space

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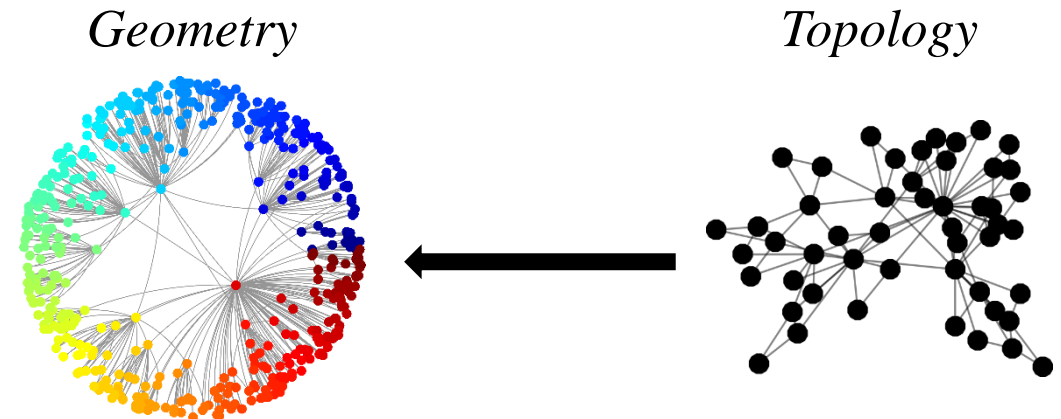
Local-ring network automata and the impact of hyperbolic geometry in complex network link-prediction

Alessandro Muscoloni, Carlo Vittorio Cannistraci

(Submitted on 29 Jul 2017)

Topological link-prediction can exploit the entire network topology (global methods) or only the neighbourhood (local methods) of the link to predict. Global methods are believed the best. Is this common belief well-founded? Stochastic-Block-Model (SBM) is a global method believed as one of the best link-predictors, therefore it is considered a reference for comparison. But, our results suggest that SBM, whose computational time is high, cannot in general overcome the Cannistraci-Hebb (CH) network automaton model that is a simple local-learning-rule of topological self-organization proved as the current best local-based and parameter-free deterministic rule for link-prediction. To elucidate the reasons of this unexpected result, we formally introduce the notion of local-ring network automata models and their relation with the nature of common-neighbours' definition in complex network theory. After extensive tests, we recommend Structural-Perturbation-Method (SPM) as the new best global method baseline. However, even SPM overall does not outperform CH and in several evaluation frameworks we astonishingly found the opposite. In particular, CH was the best predictor for synthetic networks generated by the Popularity-Similarity-Optimization (PSO) model, and its performance in PSO networks with community structure was even better than using the original internode-hyperbolic-distance as link-predictor. Interestingly, when tested on non-hyperbolic synthetic networks the

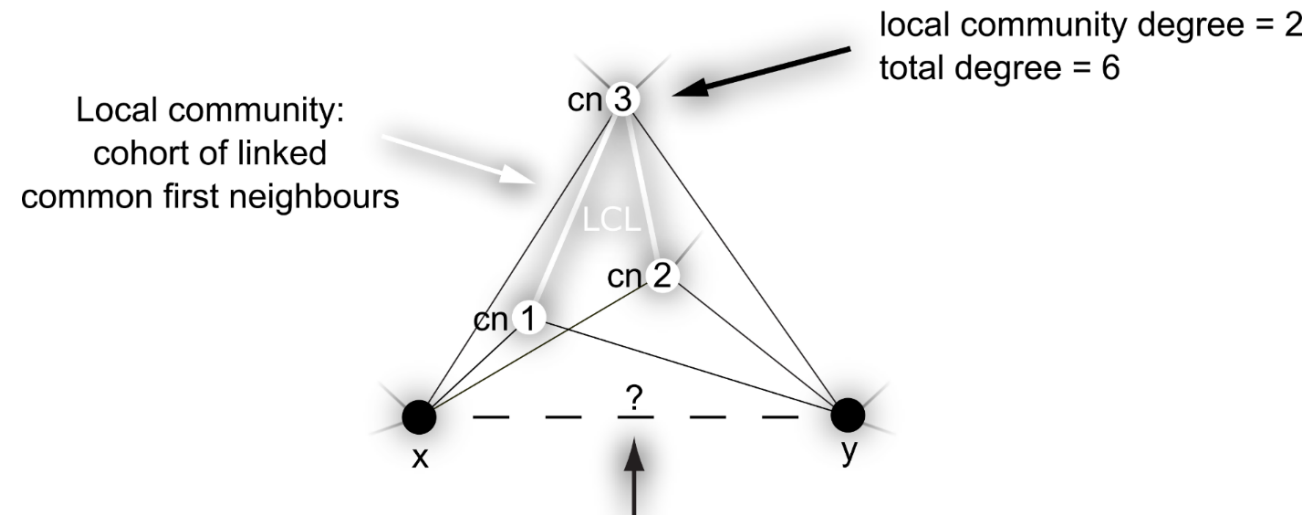
How topology predict geometry





Topological Automata: local rules that create collective intelligence

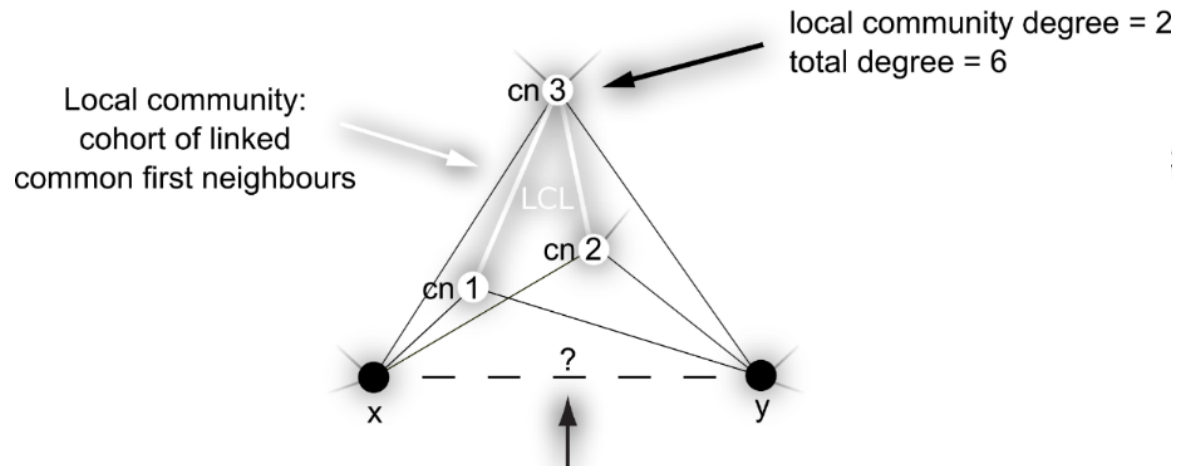
Epitopological learning on networks



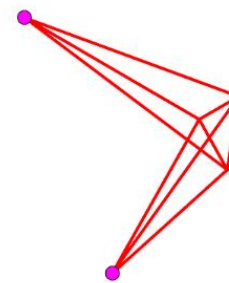
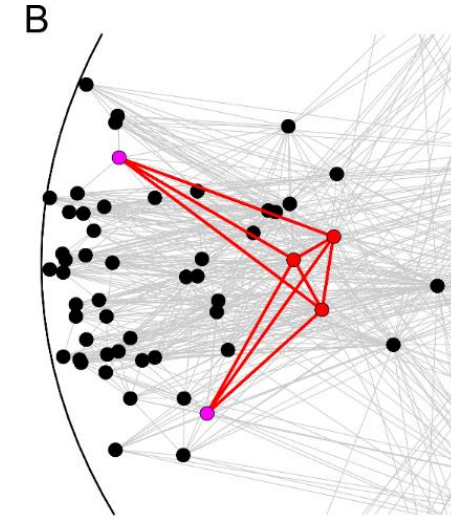
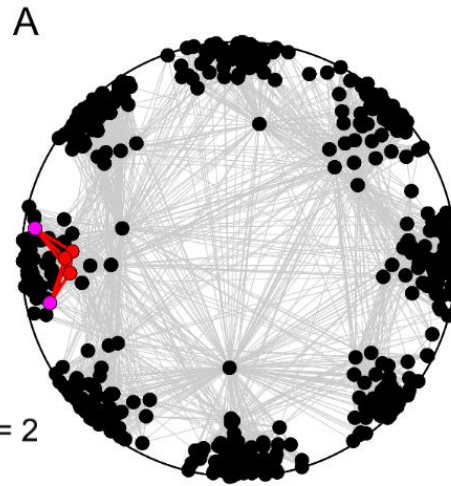
$$CRA(x, y) = \sum_{i \in CN} \frac{\text{local community degree}(i)}{\text{total degree}(i)} = \frac{1}{3} + \frac{1}{4} + \frac{2}{6} = \frac{11}{12}$$

Local-ring network automata and the impact of hyperbolic geometry in complex network link-prediction

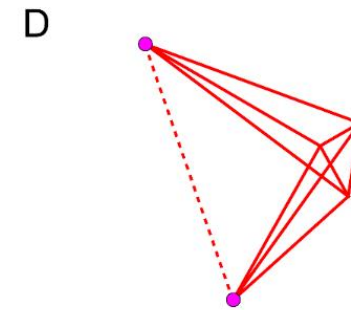
Network active/adaptive matter
Geometry and Self-organization



$$CRA(x, y) = \sum_{i \in CN} \frac{\text{local community degree}(i)}{\text{total degree}(i)} = \frac{1}{3} + \frac{1}{4} + \frac{2}{6} = \frac{11}{12}$$

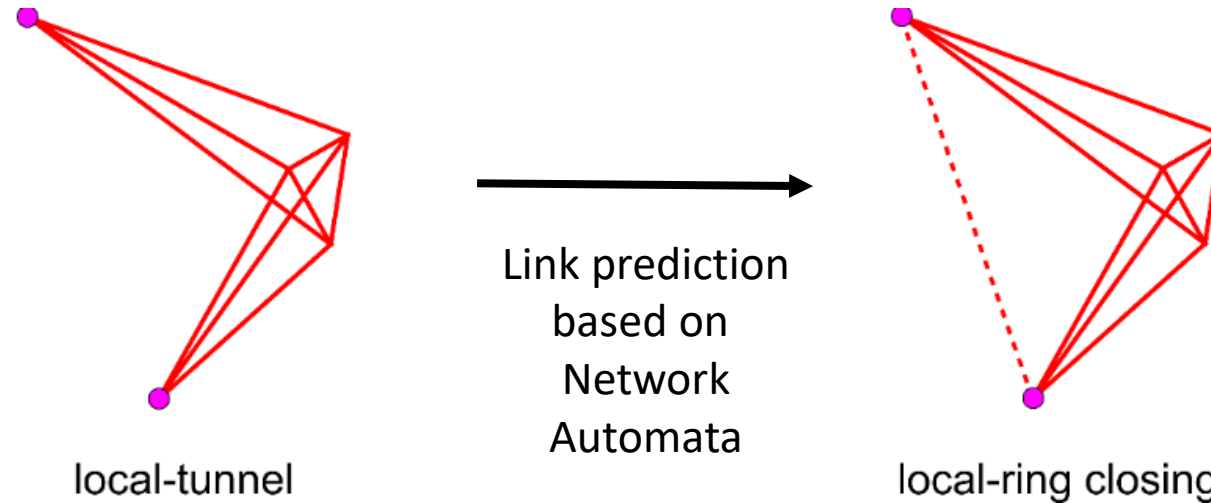


local-tunnel



local-ring closing

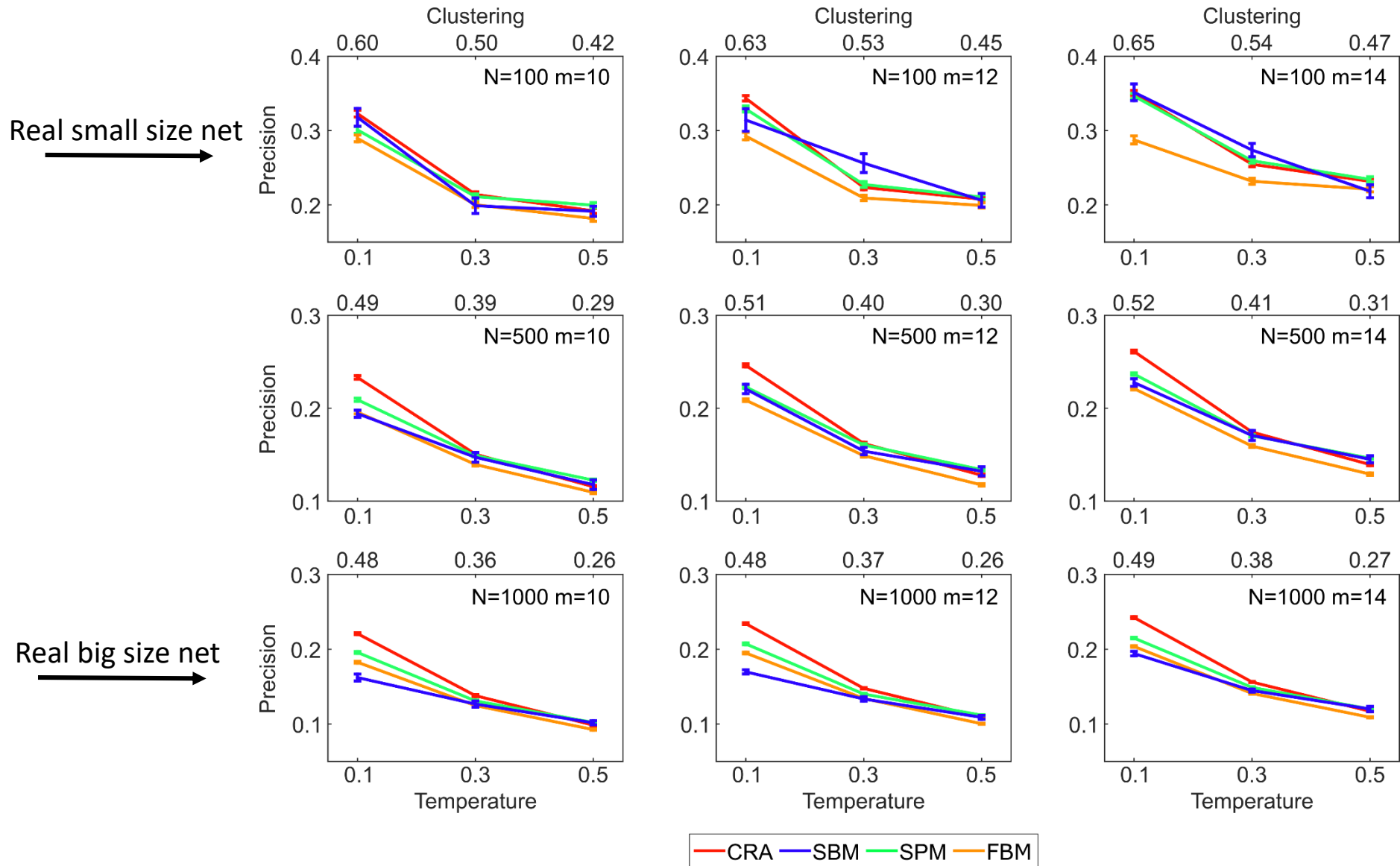
Interpretation of local similarity indices as local-ring network automata



CNs index is a network automaton that evaluates the **size** of the local tunnel to estimate the likelihood to form a local ring

CRA index is a network automaton that evaluates the **size** and assess the **existence** of the local tunnel to estimate the likelihood to form a local ring

Missing links test: 10% removal on nPSO model with 8 communities synthetic networks



Missing links test: 10% removal test on **large** networks, till 40.000 nodes

	CRA	SPM
odlis	0.12	0.08
advogato	0.16	0.15
arxiv astroph	0.53	0.67
thesaurus	0.08	0.07
arxiv hepth	0.22	0.27
ARK201012	0.16	0.11
facebook	0.11	0.10
	0.20	0.21
mean ranking	1.29	1.71
p-value	0.013	

Result: 5/7 for CRA

Link prediction in time - test (15 predictions in total on 6 nets) on *ARK-2009-09 to ARK-2010-12* Internet networks (20.000 to 30.000 nodes)

Internet networks t1 → Internet networks t2

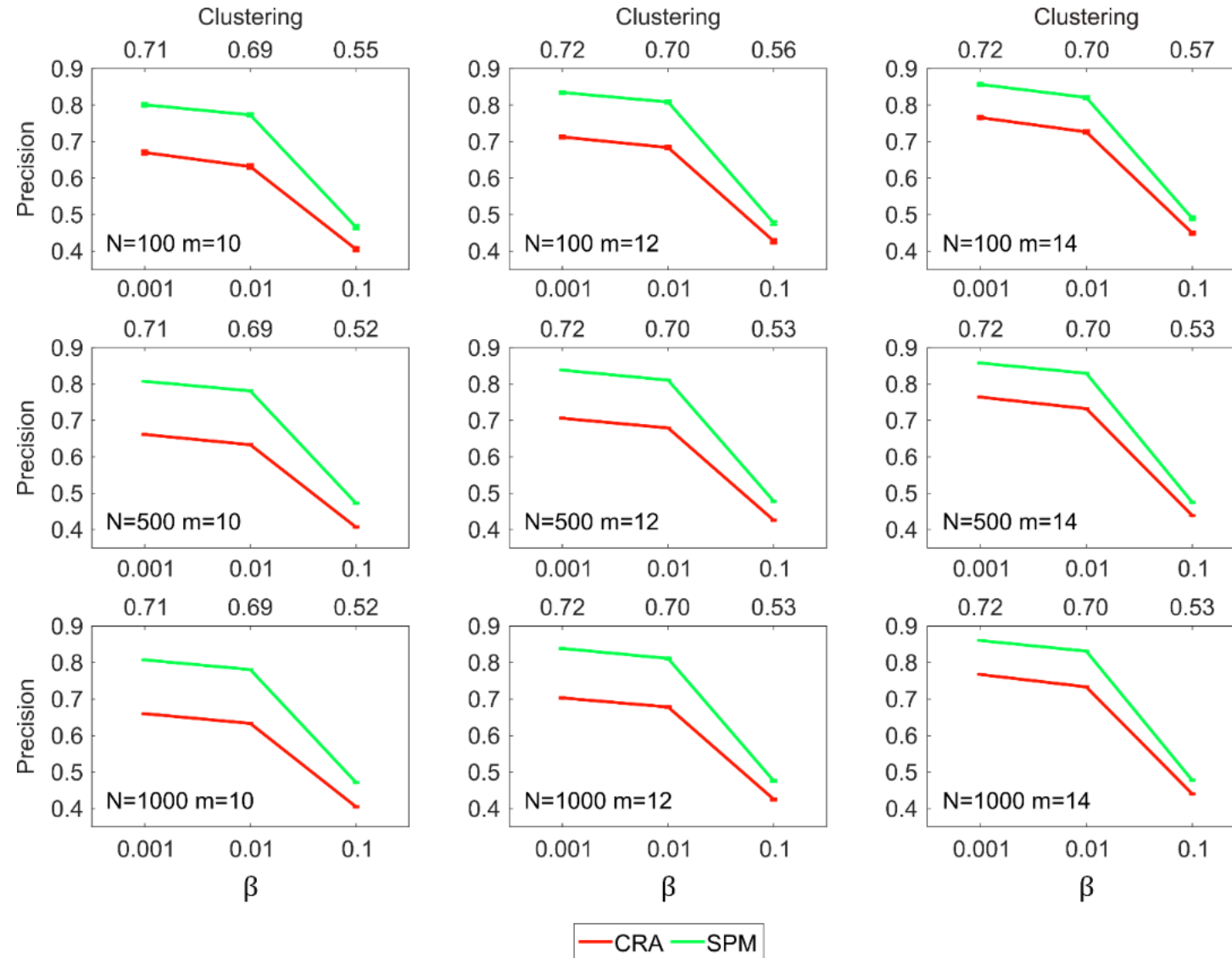
Internet networks t1 → Internet networks t3

...

Internet networks t1 → Internet networks t6

CRA						SPM						mean precision	mean ranking	mean time
	t2	t3	t4	t5	t6	t1	t2	t3	t4	t5				
t1	0.11	0.12	0.13	0.14	0.14	0.08	0.09	0.09	0.10	0.11	CRA	0.13	1	1.2 h
t2		0.12	0.13	0.14	0.14		0.07	0.08	0.09	0.10	SPM	0.09	2	6.8 h
t3			0.12	0.13	0.14			0.08	0.09	0.10				
t4				0.12	0.13				0.08	0.09				
t5					0.12					0.09				

Missing links test: 10% removal on *WS* model (which is not power-law) synthetic networks





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Local-community network automata modelling based on length-three-paths for prediction of complex network structures in protein interactomes, food webs and more

 Alessandro Muscoloni, Ilyes Abdelhamid,  Carlo Vittorio Cannistraci

doi: <https://doi.org/10.1101/346916>

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Adaptive Network Automata Modelling of Complex Networks

December 2020

[Alessandro Muscoloni](#), [Umberto Michieli](#), [Carlo Vittorio Cannistraci](#) * 

Version 1 : Received: 31 December 2020 / Approved: 31 December 2020 / Online: 31 December 2020 (13:15:22 CET)

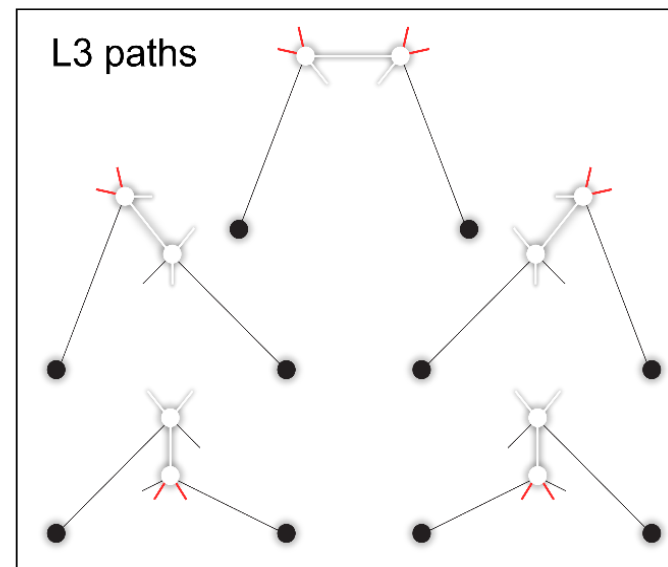
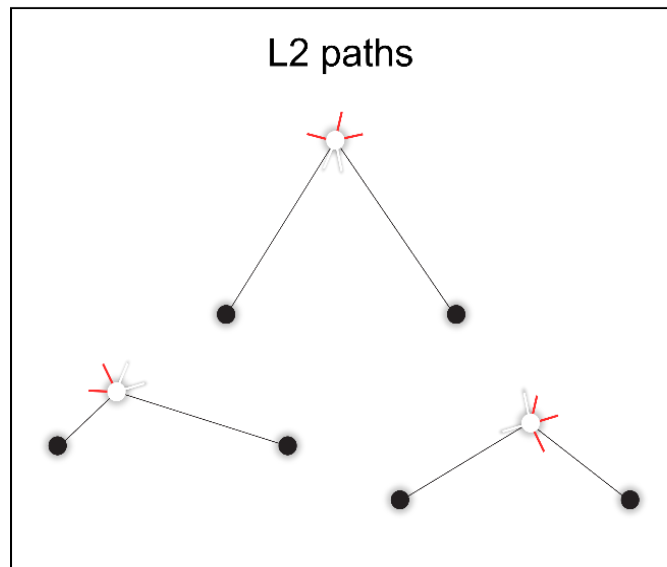
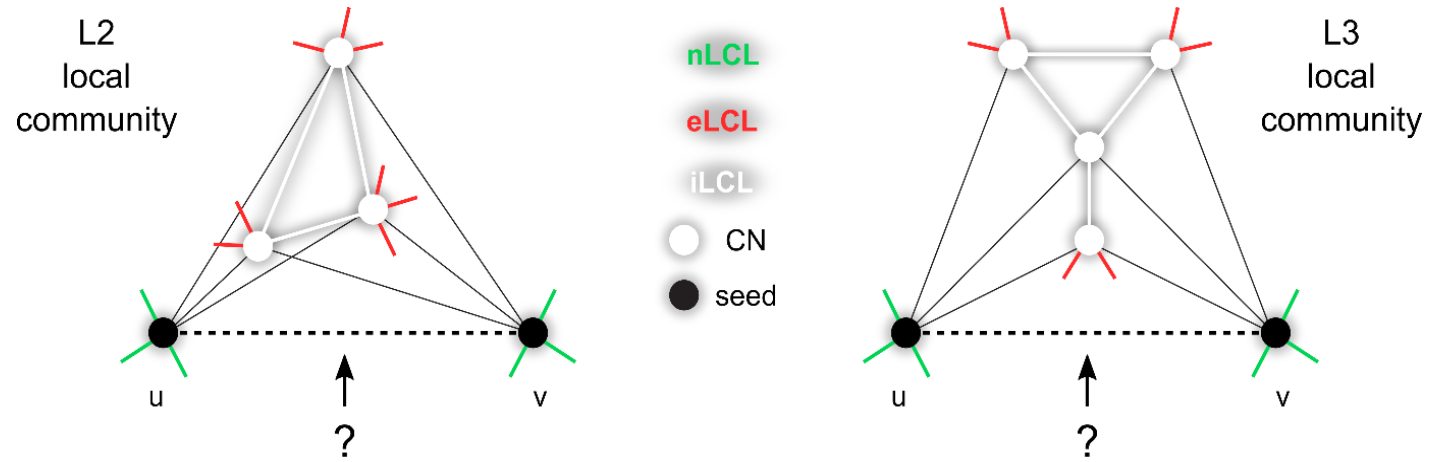
How to cite: Muscoloni, A.; Michieli, U.; Cannistraci, C.V. Adaptive Network Automata Modelling of Complex Networks. *Preprints* **2020**, 2020120808 (doi: 10.20944/preprints202012.0808.v1). [Copy](#)

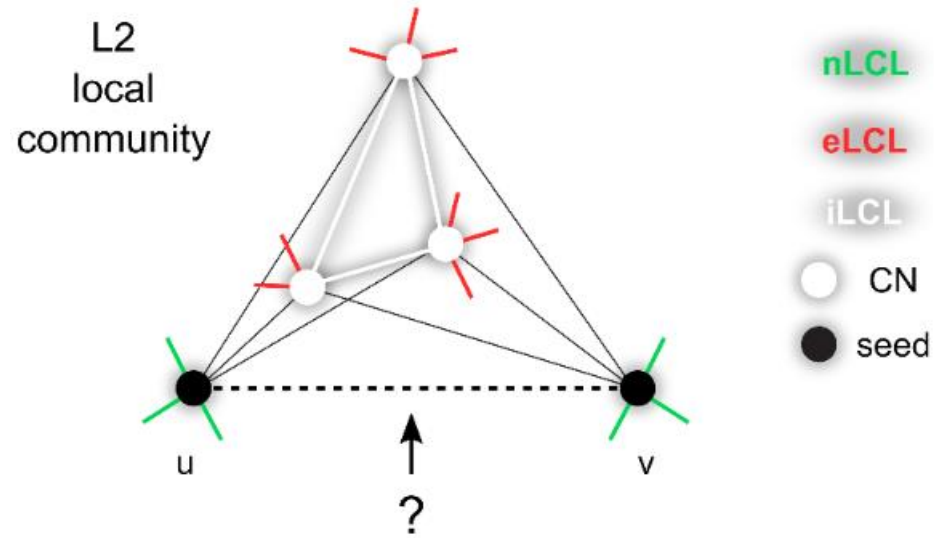
Abstract

Many complex networks have a connectivity that might be only partially detected or that tends to grow over time, hence the prediction of non-observed links is a fundamental problem in network science. The aim of topological link prediction is to forecast these non-observed links by only exploiting features intrinsic to the network topology. It has a wide range of real applications, like suggesting friendships in social networks or predicting interactions in biological networks. The Cannistraci-Hebb theory is a recent achievement in network science that includes a theoretical framework to understand local-based link prediction on paths of length n . In this study we introduce two innovations: theory of modelling (science) and theory of realization (engineering). For the theory of modelling we first recall a definition of network automata as a general framework for modelling the growth of connectivity in complex networks. We then show that several deterministic models previously developed fall within this framework and we introduce novel network automata following the Cannistraci-Hebb rule. For the theory of realization, we present how to build adaptive network automata for link prediction, which incorporate multiple deterministic models of self-organization and automatically choose the rule that better explains the patterns of connectivity in the network under investigation. We compare Cannistraci-Hebb adaptive (CHA) network automaton against state-of-the-art link prediction methods such as structural perturbation method (SPM), stochastic block models (SBM) and artificial intelligence algorithms for graph embedding. CHA displays an overall higher link prediction performance across different evaluation frameworks on 1386 networks. Finally, we highlight that CHA offers the key advantage to explicitly explain the mechanistic rule of self-organization which leads to the link prediction performance, whereas SPM and graph embedding not. In comparison to CHA, SBM unfortunately shows irrelevant and unsatisfactory performance demonstrating that SBM modelling is not adequate for link prediction in real networks.

Subject Areas

complex networks; network models; link prediction; automata theory; network automata; Cannistraci-Hebb theory

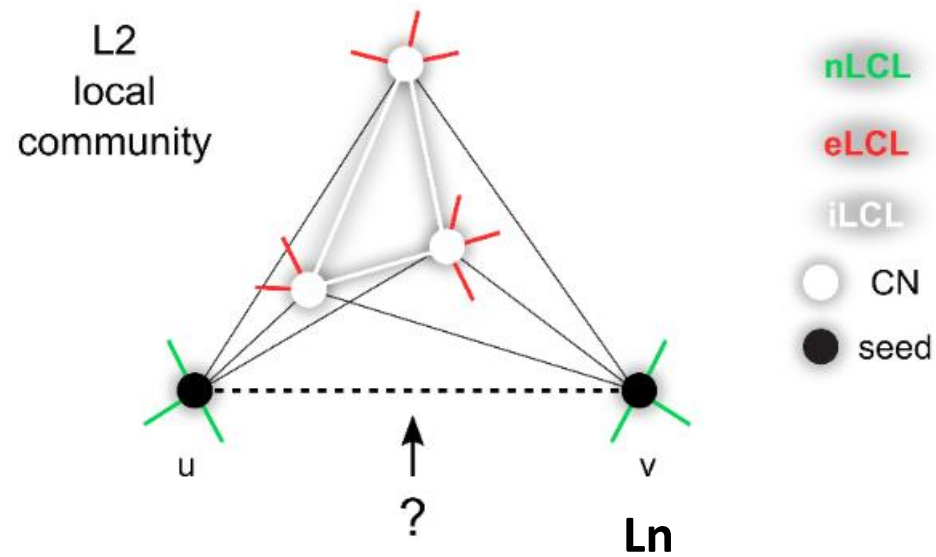




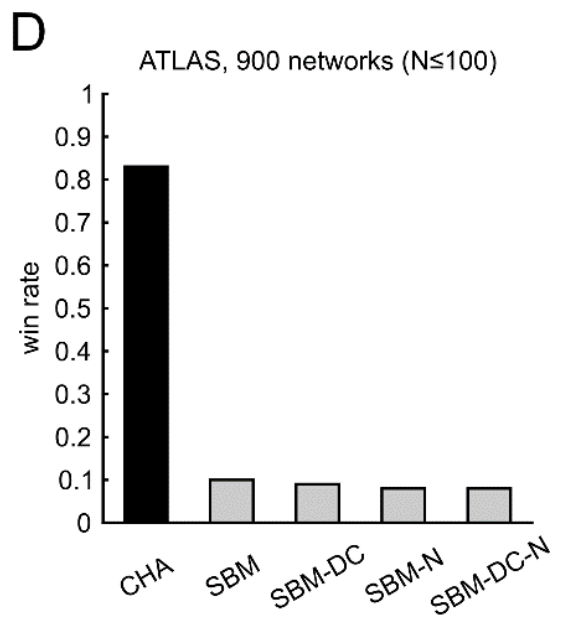
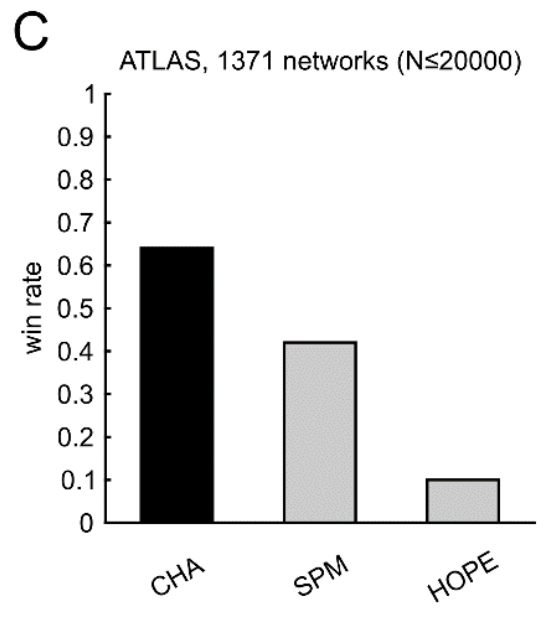
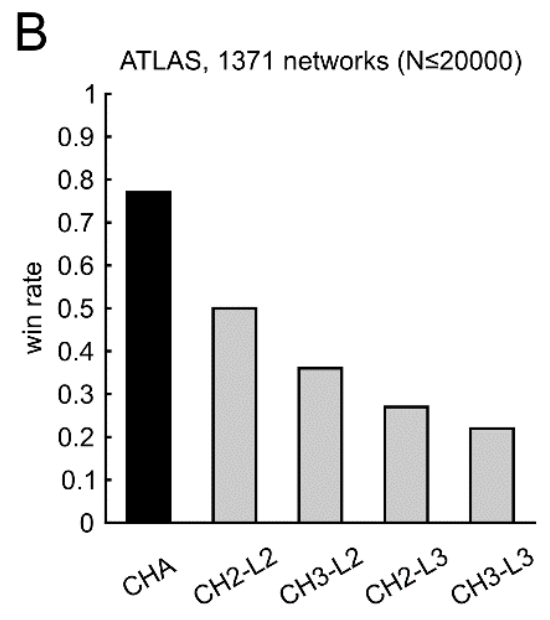
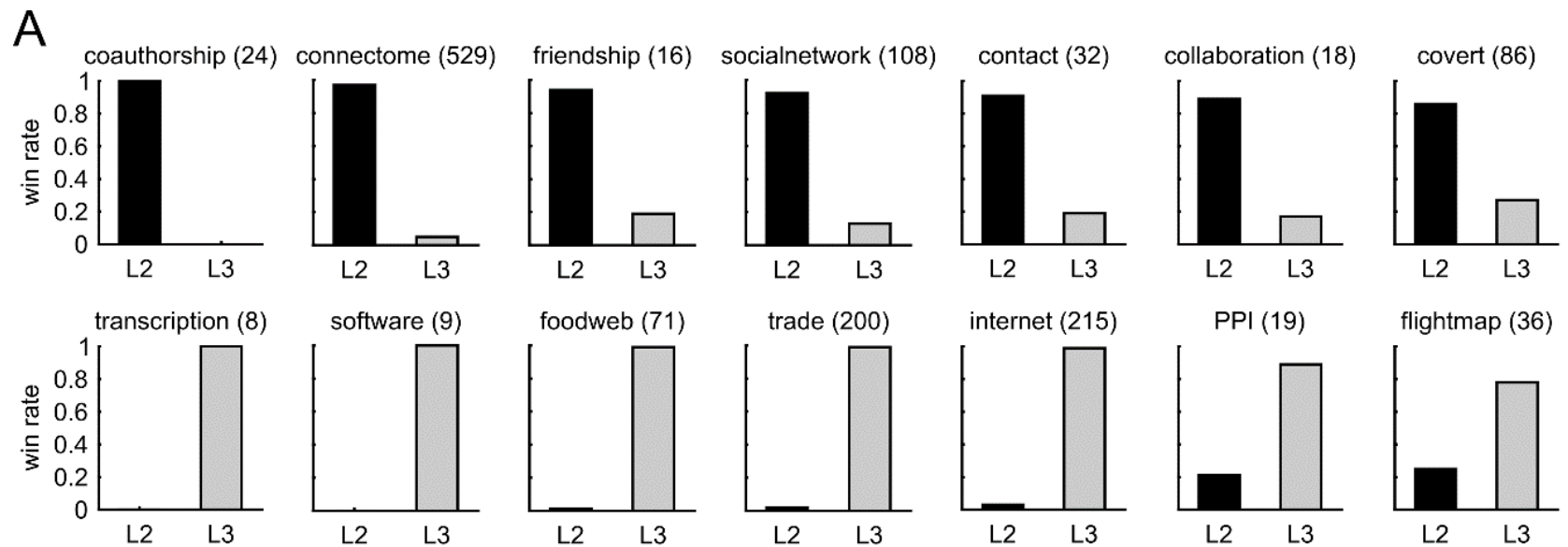
$$CRA_{L2(u,v)} = CH1_{L2(u,v)} = \sum_{z \in l2(u,v)} \frac{di_z}{d_z} = \sum_{z \in l2(u,v)} \frac{di_z}{2 + di_z + de_z} \xrightarrow{di_z \gg 2} \sum_{z \in l2(u,v)} \frac{1}{1 + de_z/di_z}$$

Network Automata

- CH1 and CH2: minimization of the eLCL and maximization of the iLCL.
- CH3 solely based on the minimization of eLCL.



L2	L3	Ln
$CH1_{L2}(u, v) = \sum_{z \in L2} \frac{di_z}{d_z}$	$CH1_{L3}(u, v) = \sum_{z_1, z_2 \in L3} \frac{\sqrt{di_{z_1} * di_{z_2}}}{\sqrt{d_{z_1} * d_{z_2}}}$	$CH1_{Ln}(u, v) = \sum_{z_1 \dots z_{n-1} \in Ln} \frac{(di_{z_1} * \dots * di_{z_{n-1}})^{\frac{1}{n-1}}}{(d_{z_1} * \dots * d_{z_{n-1}})^{\frac{1}{n-1}}}$
$CH2_{L2}(u, v) = \sum_{z \in L2} \frac{di_z^*}{de_z^*}$	$CH2_{L3}(u, v) = \sum_{z_1, z_2 \in L3} \frac{\sqrt{di_{z_1}^* * di_{z_2}^*}}{\sqrt{de_{z_1}^* * de_{z_2}^*}}$	$CH2_{Ln}(u, v) = \sum_{z_1 \dots z_{n-1} \in Ln} \frac{(di_{z_1}^* * \dots * di_{z_{n-1}}^*)^{\frac{1}{n-1}}}{(de_{z_1}^* * \dots * de_{z_{n-1}}^*)^{\frac{1}{n-1}}}$
$CH3_{L2}(u, v) = \sum_{z \in L2} \frac{1}{de_z^*}$	$CH3_{L3}(u, v) = \sum_{z_1, z_2 \in L3} \frac{1}{\sqrt{de_{z_1}^* * de_{z_2}^*}}$	$CH3_{Ln}(u, v) = \sum_{z_1 \dots z_{n-1} \in Ln} \frac{1}{(de_{z_1}^* * \dots * de_{z_{n-1}}^*)^{\frac{1}{n-1}}}$



Experimental analyses on 2-hop-based and 3-hop-based link



Tao Zhou

Web Sciences Center

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networks human dynamics recommendation prediction

2020

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of known methods are similarity-based, which assign similarity indices for node pairs and assume that two nodes of larger similarity have higher probability to be connected

: majority


2-hop-based and 3-hop-based similarity indices on 137 real networks. Overall speaking, the class of Cannistraci–Hebb indices performs the best among all considered candidates.

2-hop-based and 3-hop-based similarity indices on 137 real networks. Overall speaking, the class of Cannistraci–Hebb indices performs the best among all considered candidates. In addition, 3-hop-based indices outperform 2-hop-based indices on ROC-AUC, and 3-hop-based indices and 2-hop-based indices are competitive on precision. Further statistical results show that 3-hop-based indices are more suitable for disassortative networks with lower densities and lower average clustering coefficients.

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Highly accurate protein structure prediction with AlphaFold

[John Jumper](#) , [Richard Evans](#), [Alexander Pritzel](#), [Tim Green](#), [Michael Figurnov](#), [Olaf Ronneberger](#), [Kathryn Tunyasuvunakool](#), [Russ Bates](#), [Augustin Židek](#), [Anna Potapenko](#), [Alex Bridgland](#), [Clemens Meyer](#), [Simon A. Kohl](#), [Andrew J. Ballard](#), [Andrew Cowie](#), [Bernardino Romera-Paredes](#), [Stanislav Nikolov](#), [Rishub Jain](#), [Jonas Adler](#), [Trevor Back](#), [Stig Petersen](#), [David Reiman](#), [Ellen Clancy](#), [Michal Zielinski](#), ... [Demis Hassabis](#) 

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Abstract

Proteins are essential to life, and understanding their structure can facilitate a mechanistic understanding of their function. Through an enormous experimental effort^{1,2,3,4}, the

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Kathryn Tunyasuvunakool, Jonas Adler ... Demis Hassabis
Nature | **Article** | [Open Access](#) | 22 Jul 2021

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Protein complex prediction with AlphaFold-Multimer

Richard Evans, Michael O'Neill, Alexander Pritzel, Natasha Antropova, Andrew Senior, Tim Green, Augustin Židek, Russ Bates, Sam Blackwell, Jason Yim, Olaf Ronneberger, Sebastian Bodenstern, Michal Zielinski, Alex Bridgland, Anna Potapenko, Andrew Cowie, Kathryn Tunyasuvunakool, Rishub Jain, Ellen Clancy, Pushmeet Kohli, John Jumper, Demis Hassabis

doi: <https://doi.org/10.1101/2021.10.04.463034>

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Abstract

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Abstract

While the vast majority of well-structured single protein chains can now be predicted to high accuracy due to the recent AlphaFold [1] model, the prediction of multi-chain protein complexes remains a challenge in many cases. In this work, we demonstrate that an AlphaFold model trained specifically for multimeric inputs of known stoichiometry, which we call AlphaFold-Multimer, significantly increases accuracy of

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AF2Complex predicts direct physical interactions in multimeric proteins with deep learning

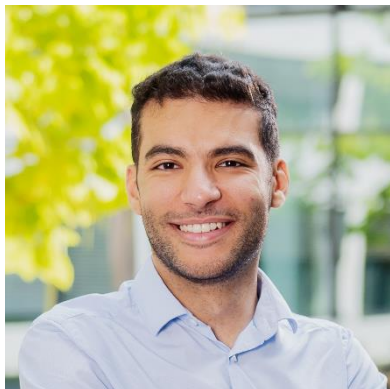
[Mu Gao](#) , [Davi Nakajima An](#), [Jerry M. Parks](#) & [Jeffrey Skolnick](#) 

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Abstract


Accurate descriptions of protein-protein interactions are essential for understanding biological systems. Remarkably accurate atomic structures have been recently computed for individual proteins by AlphaFold2 (AF2). Here, we demonstrate that the same neural network



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Network shape intelligence outperforms AlphaFold2 intelligence in vanilla protein interaction prediction

Ilyes Abdelhamid, Alessandro Muscoloni, Danny Marc Rotscher, Matthias Lieber, Ulf Markwardt,
 Carlo Vittorio Cannistraci

doi: <https://doi.org/10.1101/2023.08.10.552825>

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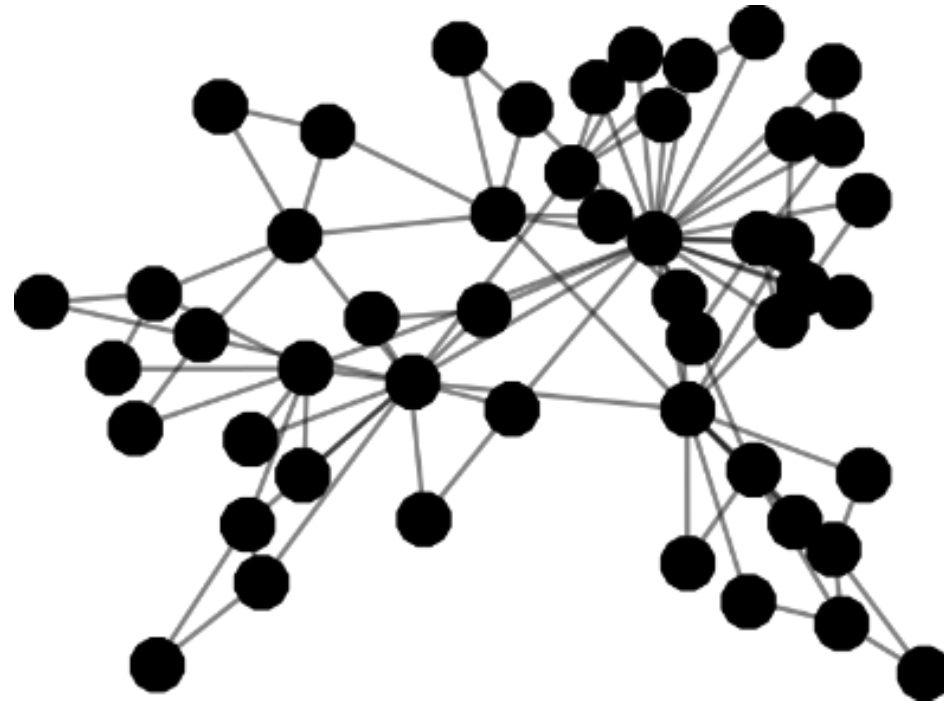
Abstract

For decades, scientists and engineers have been working to predict protein interactions, and network topology methods have emerged as extensively studied techniques. Recently, approaches based on AlphaFold2 intelligence, exploiting 3D

Nature Machine Intelligence 2023 under review

Yeast protein interaction network

4951 proteins and 22382 interactions

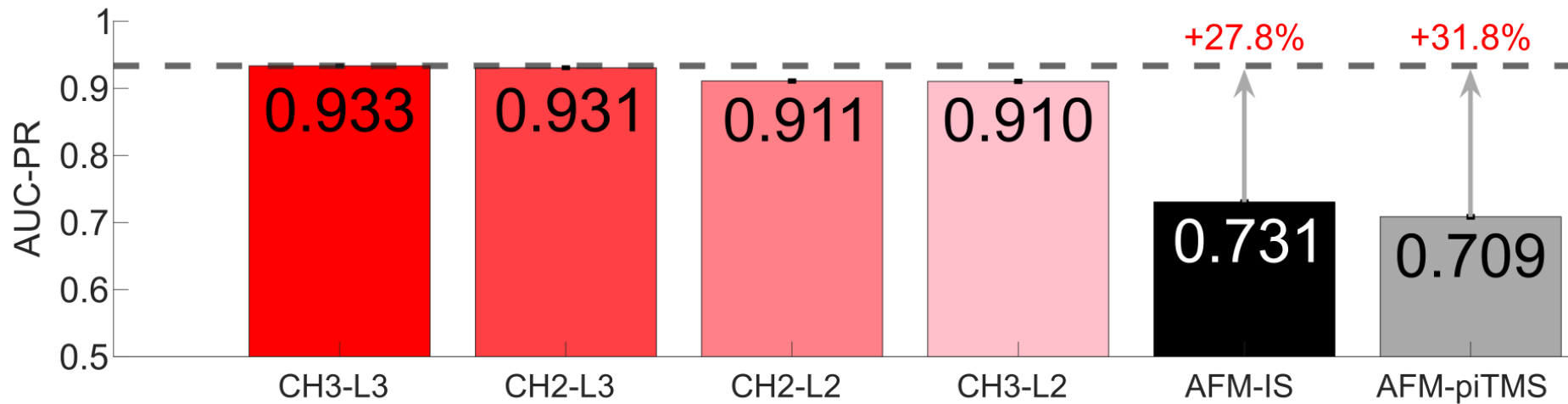
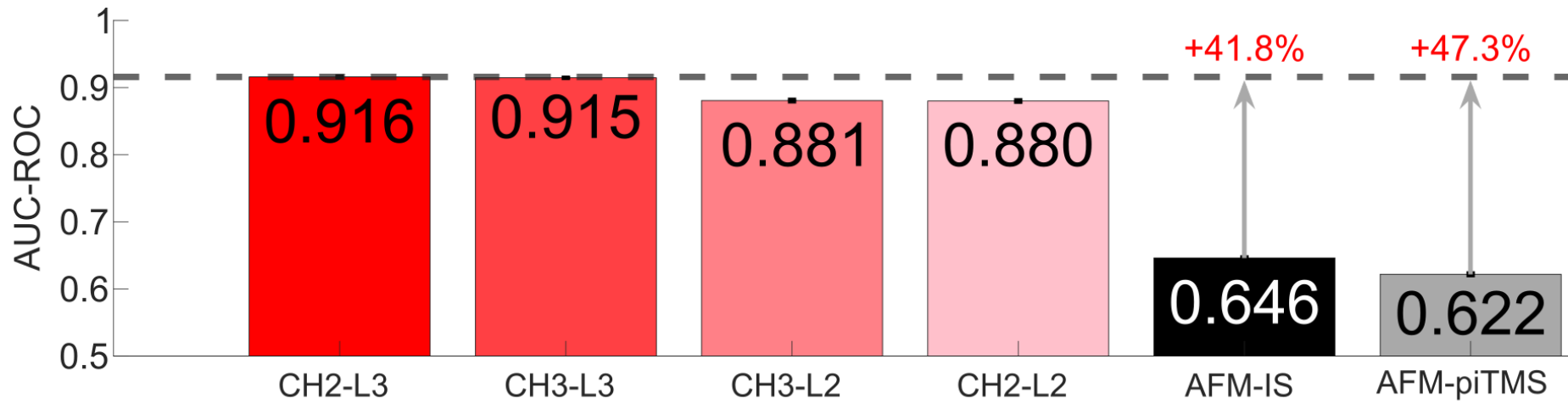


2238 (10%)

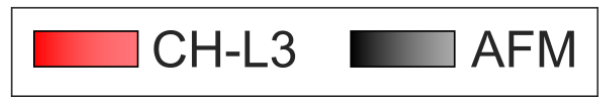
Positive interactions

2238 (10%)

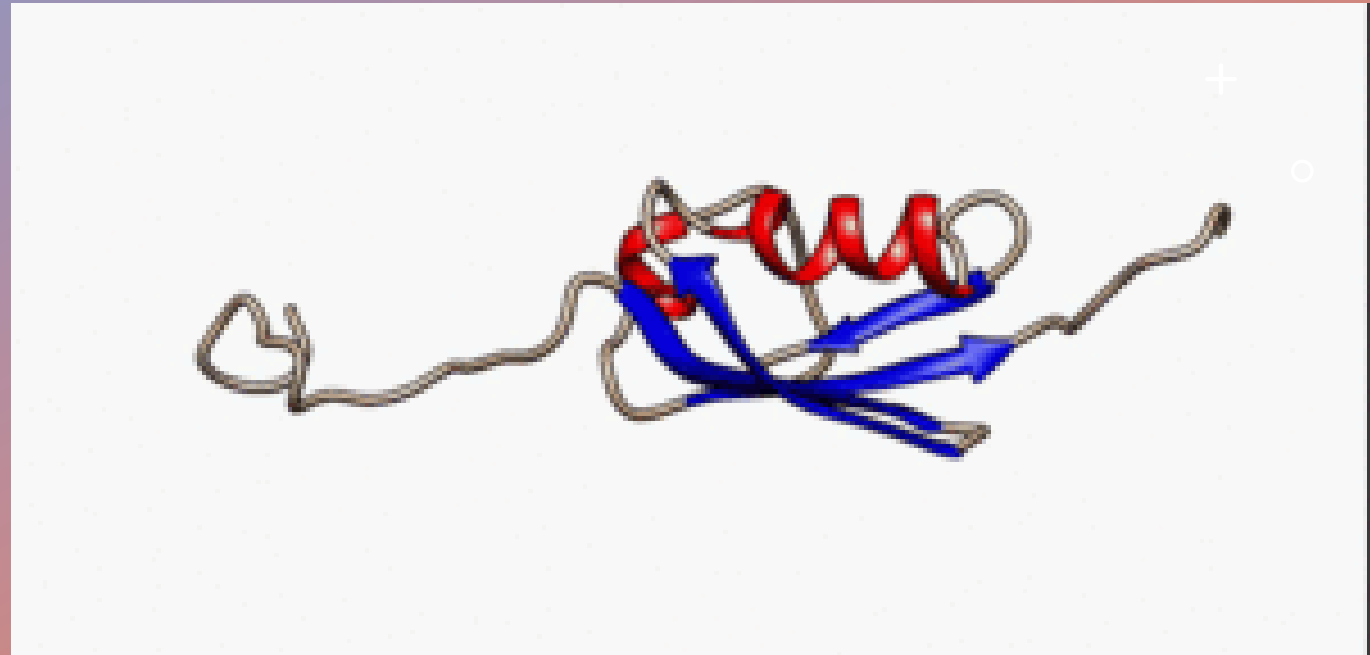
Negative interactions



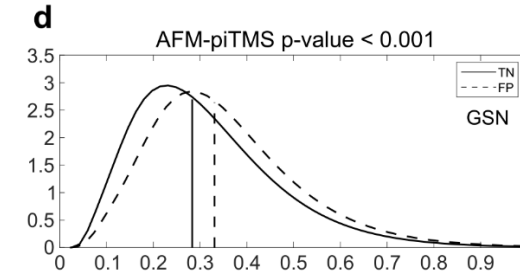
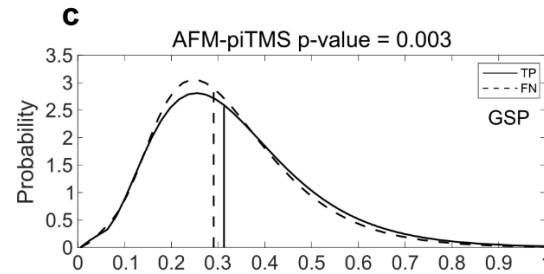
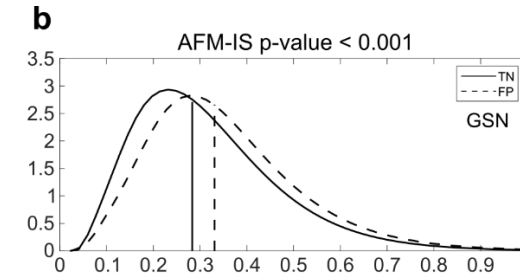
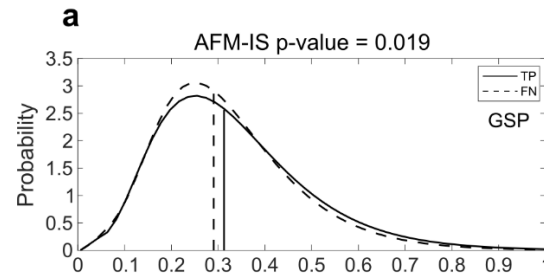
Methods



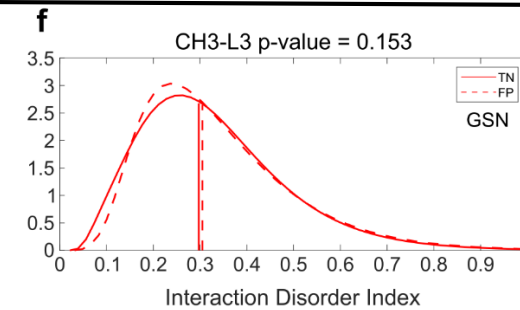
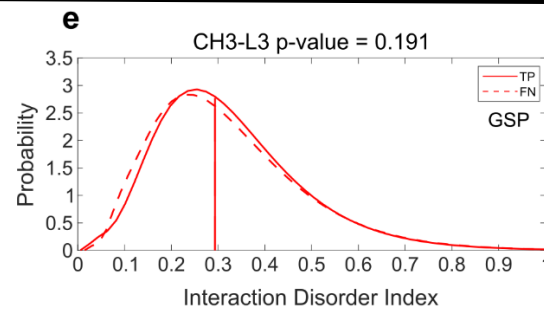
Intrinsically disordered protein



**Interaction disorder index
is significantly different
for wrong AFM predictions**

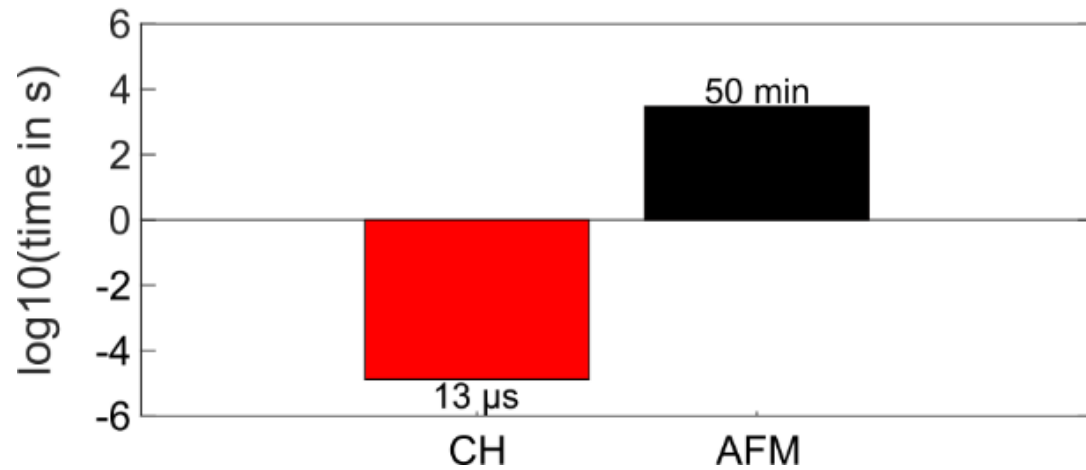


**Interaction disorder index
is not different
for wrong CH predictions**

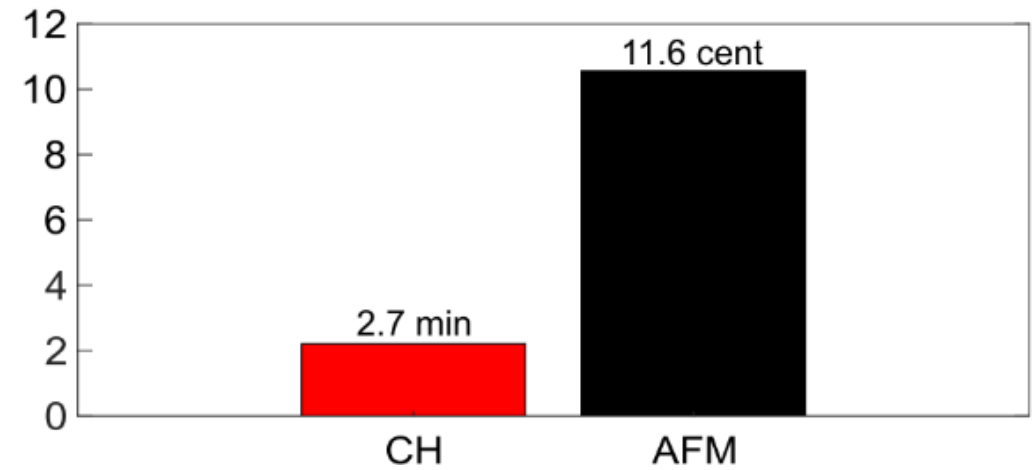


Comparison in computational running time

One interaction



All missing interactions



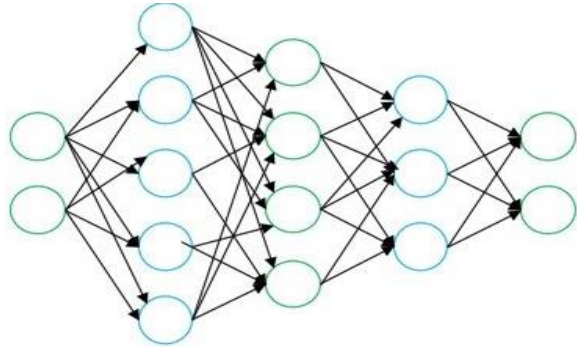
OUTLINE of the talk

1. Prediction of connectivity in sparse network structures
2. Dynamic sparse training in deep learning
3. Neuromorphic computing

Meanwhile in computer science

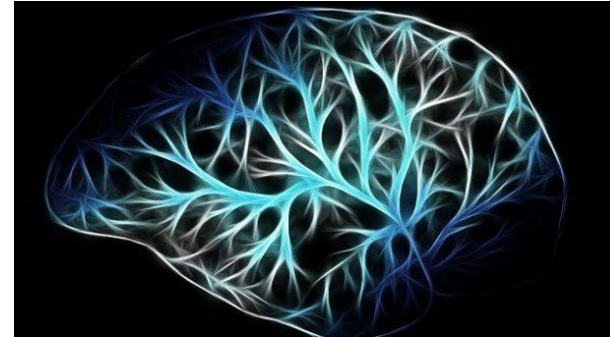
Crisis: I was a Master student in 2002

Artificial Neural Network (ANN)



Vs.

Brain Connectivity



Crisis: Why is brain connectivity sparse?

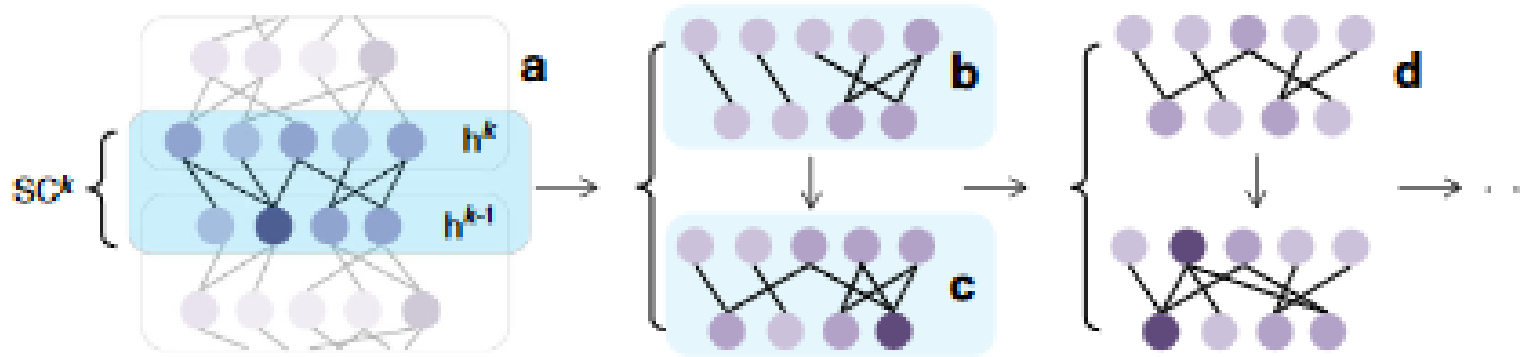
- 1. What is the computational advantage of connectivity sparsity in brain biology?*
- 2. How to make profit of brain-inspired connectivity sparsity in ANN?***

Crisis: Unacceptable Cost of Training models

- **GPT-3:** 175 billion parameters
 - **Cost (2020):** \$4.6 million
- **GPT-4 (Human Brain):** 100 trillion parameters
 - **Cost (2020):** \$2.6 billion

GPT-3 model == 1024 A100 GPUs and 34 days == 4.6 million dollars

Sparse Evolutionary Training (SET)



1. Start from a sparse connected topology given by **Erdos-Renyi model**
2. Train the network in an evolution epoch
3. Remove a certain fraction of weights with **the lowest absolute value**
4. **Randomly** regrow new weights in the same amount as the ones removed previously
5. Repeat step 2 - 4 until the network convergence

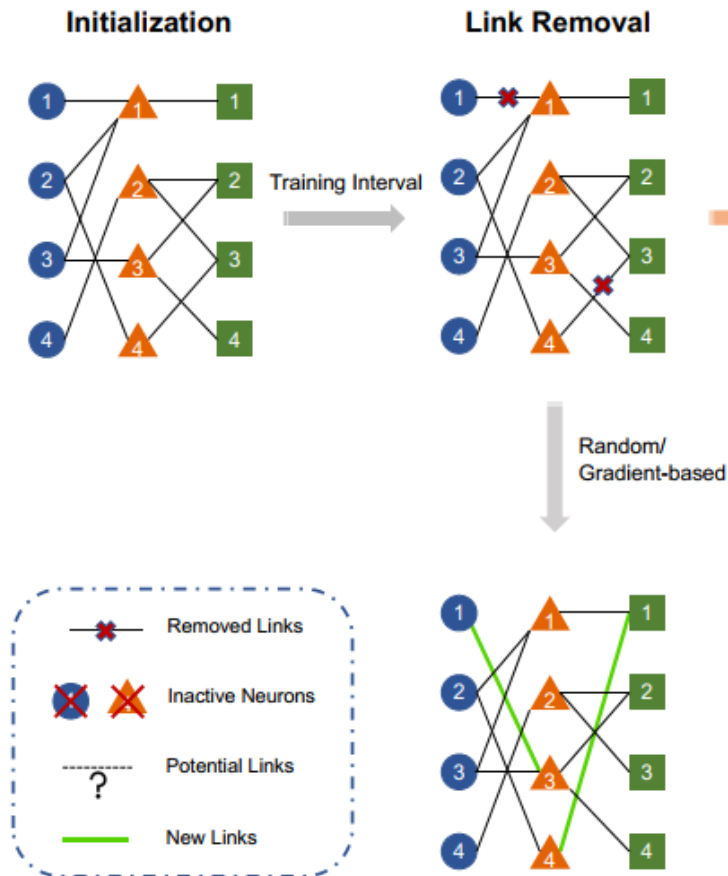
Epitopological Learning (EL)

- *a brain-inspired learning paradigm*
- *a field of network science that studies how to implement learning on networks by **changing the shape of their connectivity structure** (epitopological plasticity):*
-> *a subcase: $T^{n+1} = T^n + LP_{TopK}(T^n)$*
- *The **Cannistraci-Hebb theory** is a strategy to implement EL based on local topology information*

Epitopological Sparse Meta-Deep Learning (ESML)

Dynamic Sparse Training

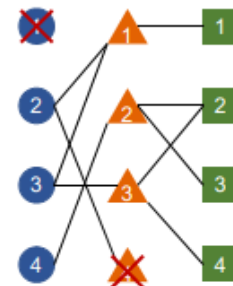
(Mocanu et al 2018 / Evci et al 2020)



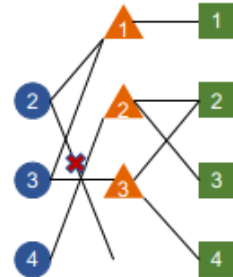
Epitopological Sparse Meta-deep Learning

Network percolation

Inactive Neurons Removal

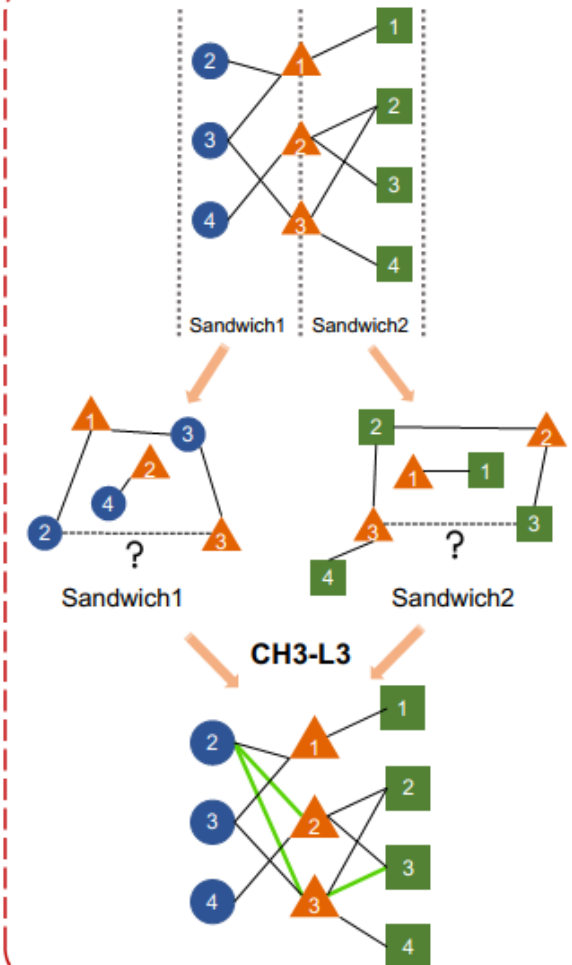


two rounds



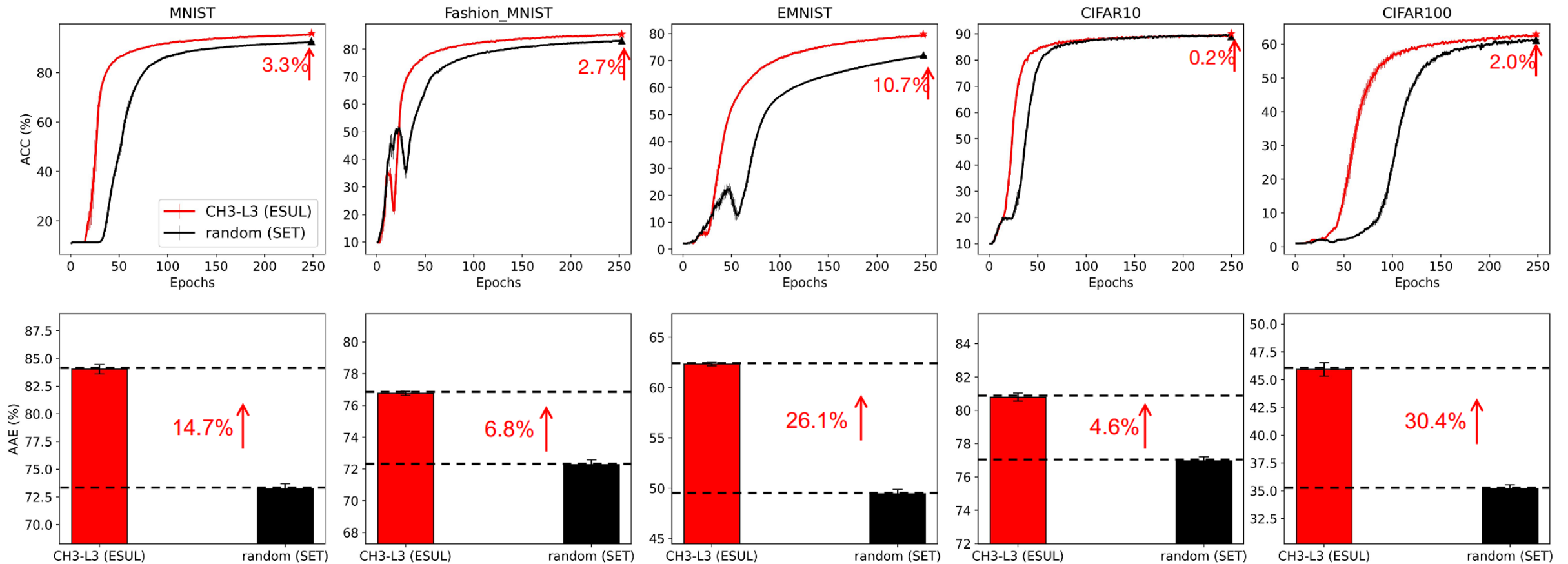
Incomplete Path Adjustment

EL (Link prediction)



Comparison of CH3-L3 (ESML) and random (SET)

Results on 5 datasets and 2 architectures



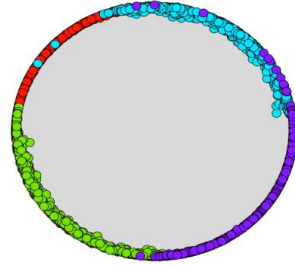
How the topology evolves during the epochs

<https://www.youtube.com/watch?v=b5lLpOhb3BI>

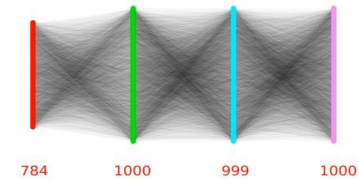
Epoch: 0

Both of the networks initialized with Erdos-Renyi network

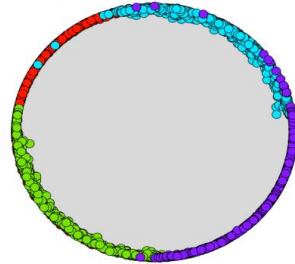
Hyperbolic presentation of SET (Random)



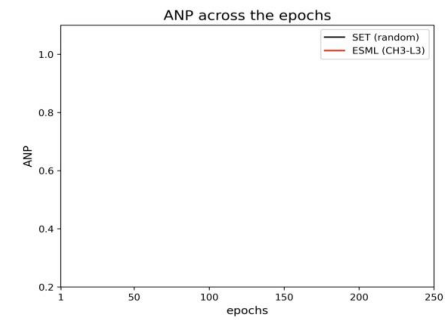
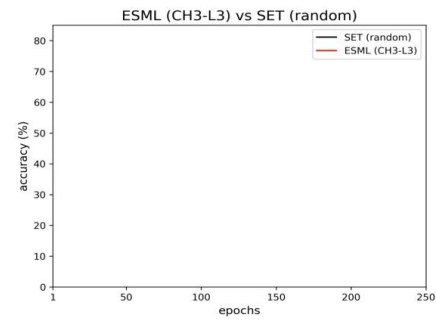
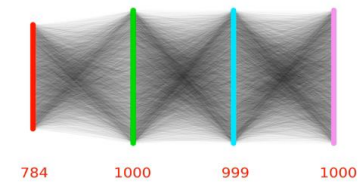
Plain presentation of SET (Random)



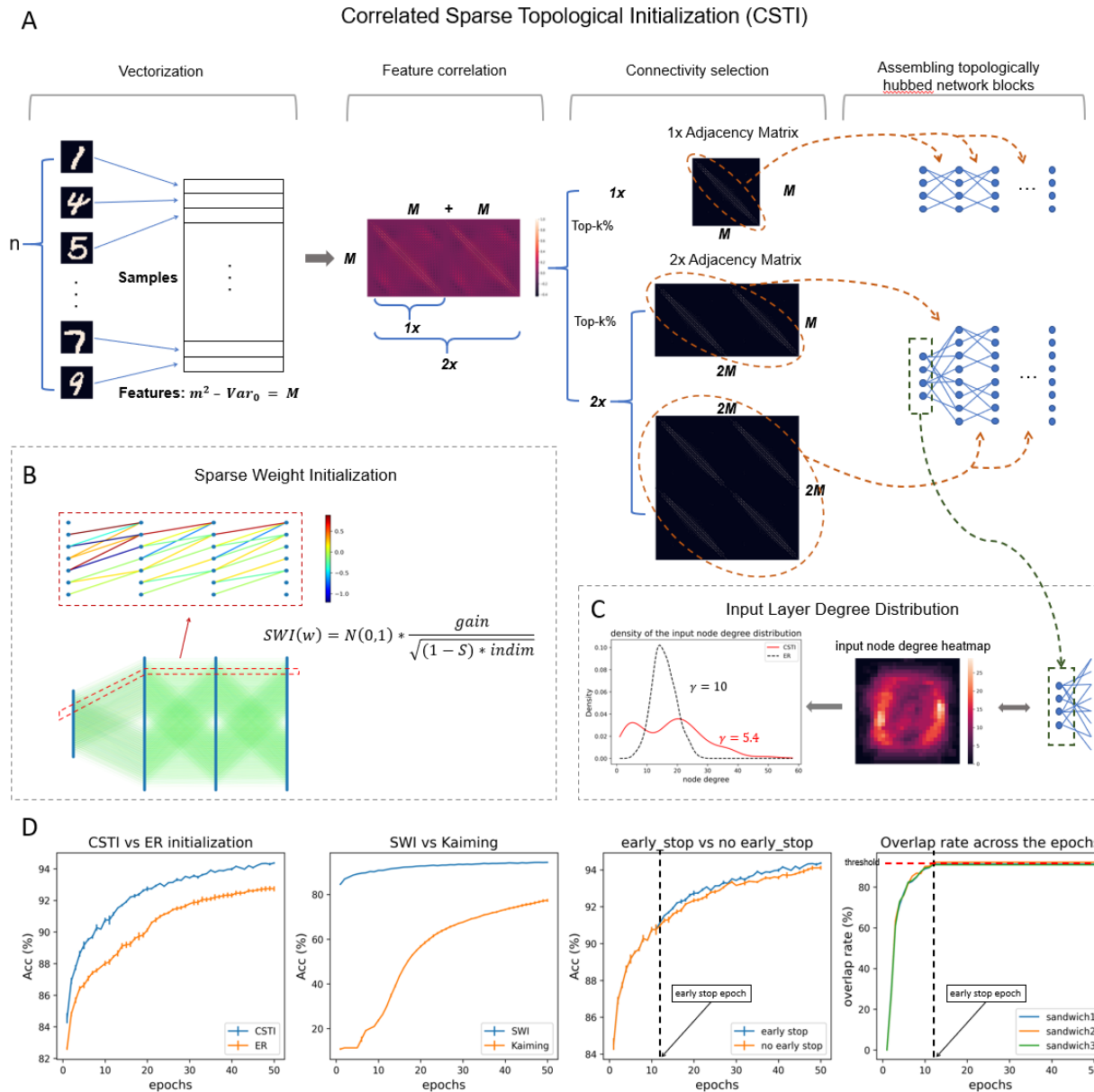
Hyperbolic presentation of ESML (CH3-L3)



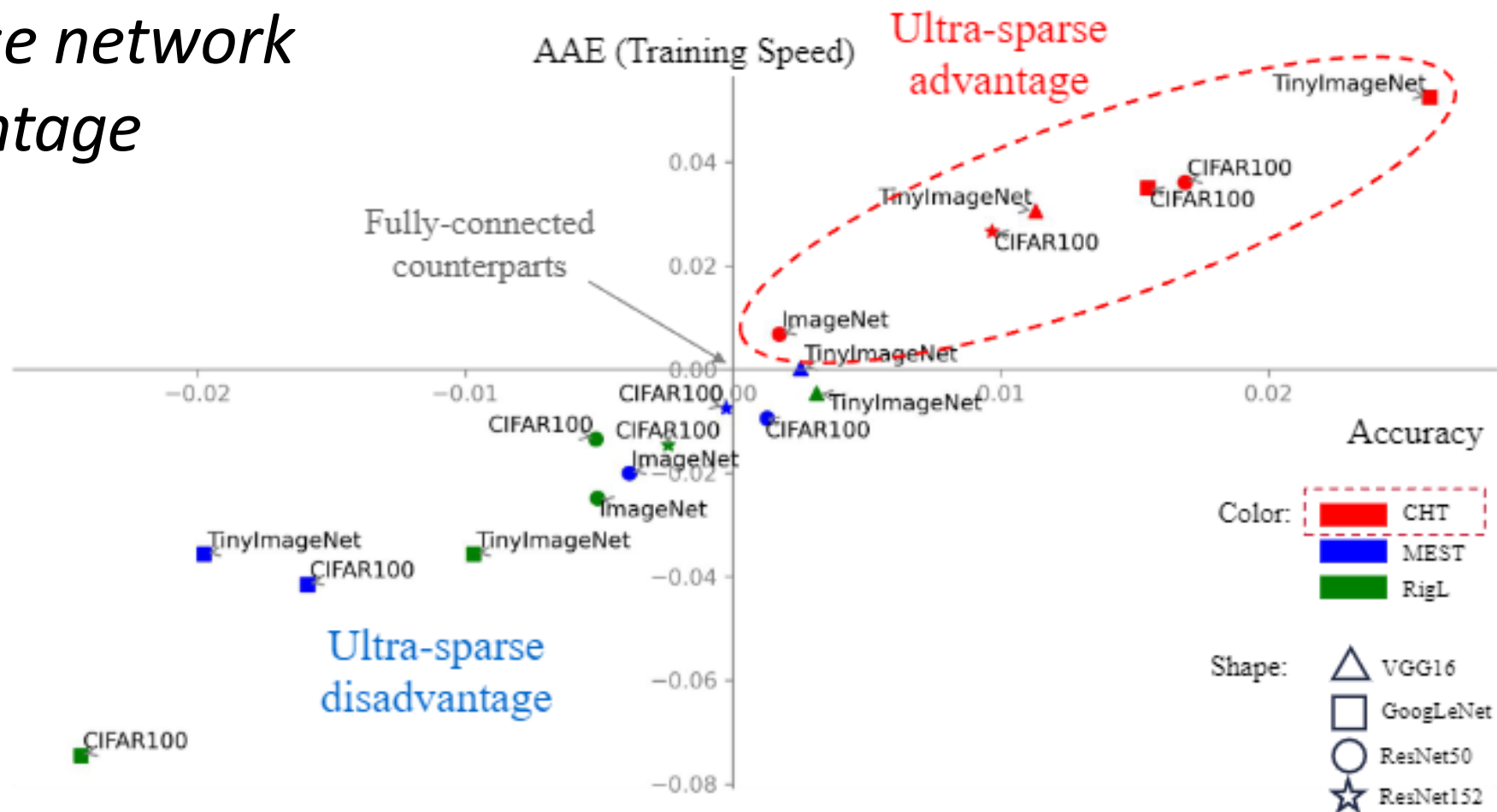
Plain presentation of ESML (CH3-L3)



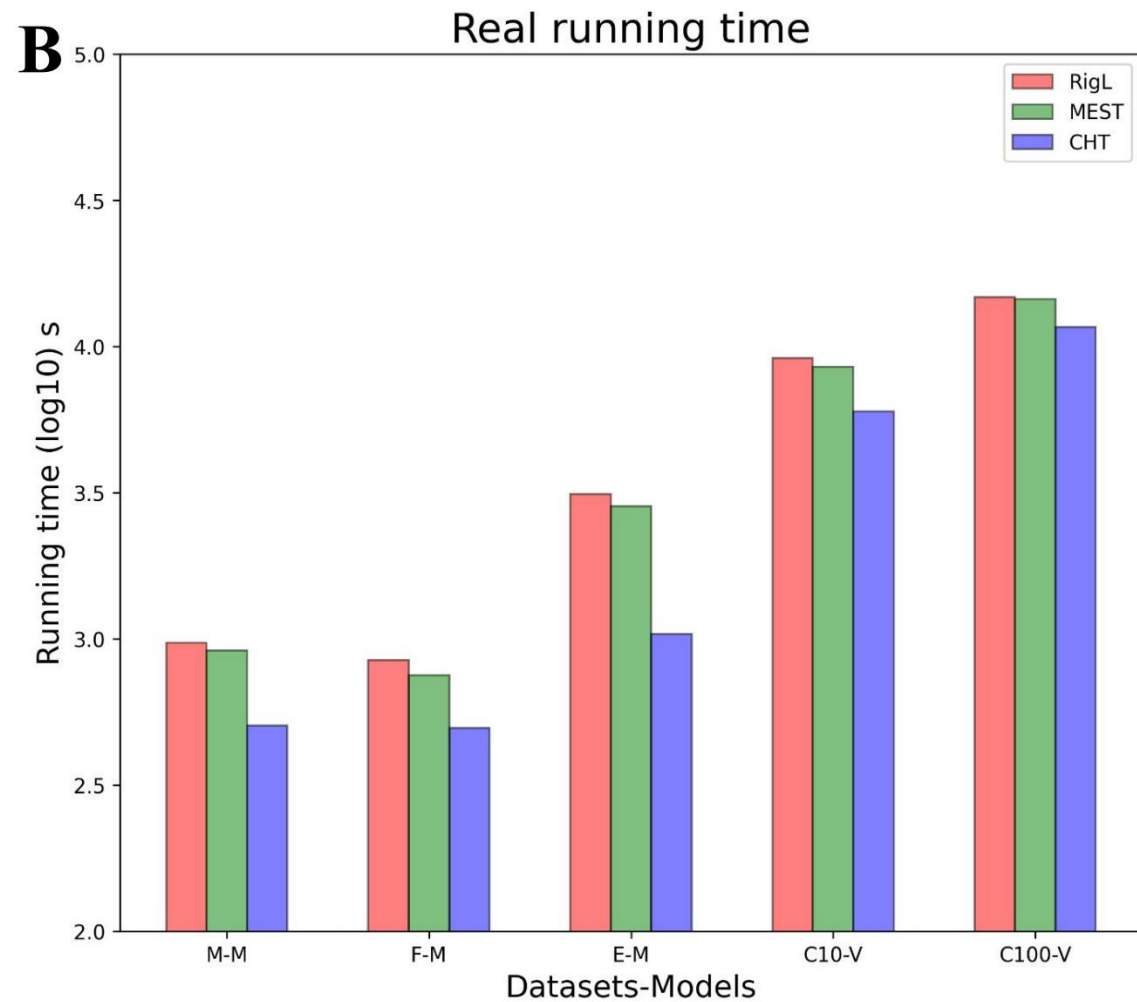
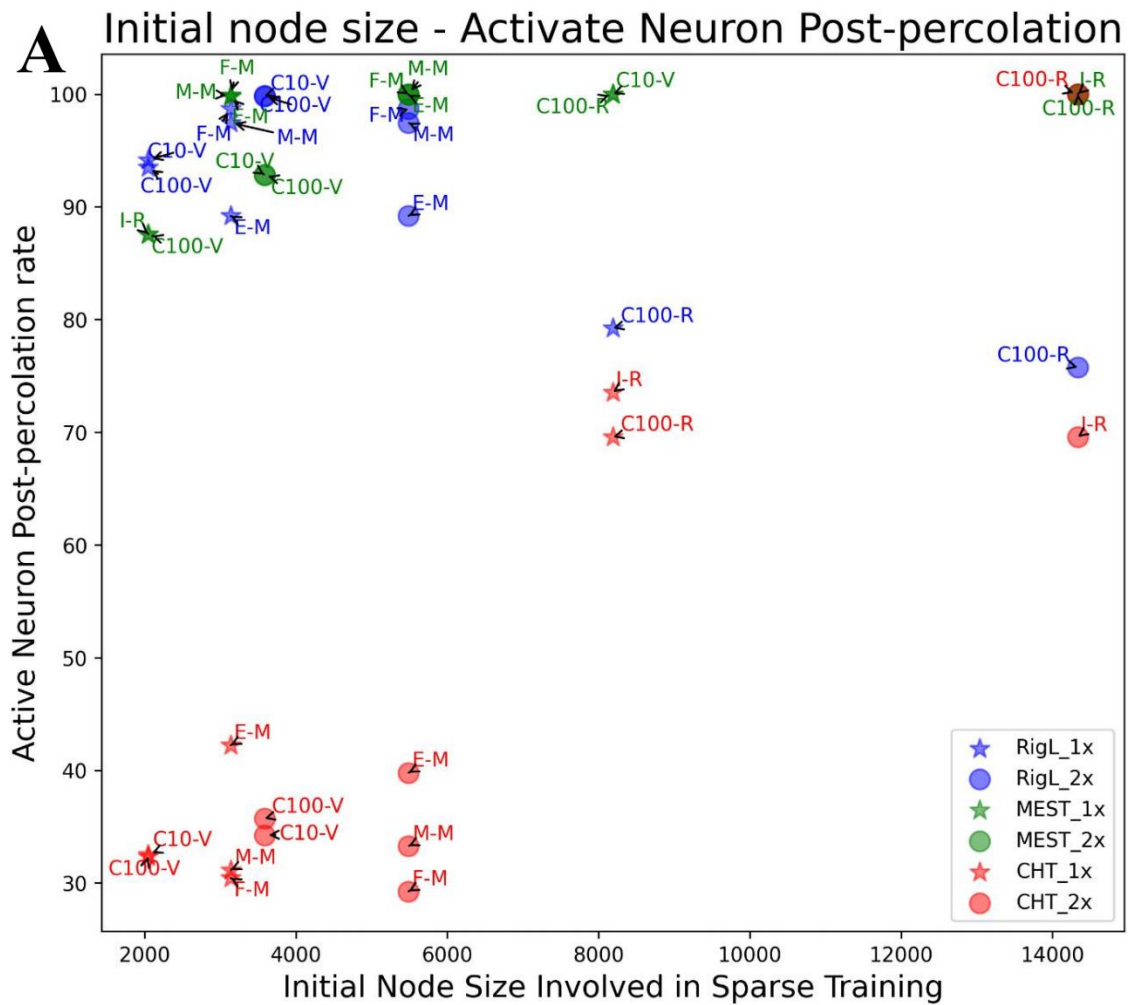
CHT innovations and their impact on performance



Ultra-sparse network advantage



	VGG16-TinyImageNet S:100K C:200		GoogLeNet-CIFAR100 S:50K C:100		GoogLeNet-TinyImageNet S:100K C:200		ResNet50-CIFAR100 S:50K C:100		ResNet50-ImageNet S:1.2M C:1000	
	ACC	AAE	ACC	AAE	ACC	AAE	ACC	AAE	ACC	AAE
FC _{1x}	51.34±0.12	43.55±0.04	76.64±0.1	62.9±0.07	52.63±0.08	45.14±0.02	78.3±0.03	65.53±0.09	75.04±0.05	63.27±0.03
RigL _{1x}	51.32±0.25	43.0±0.12	74.12±0.34	56.96±0.68	51.23±0.12	42.59±0.2	78.08±0.08	64.54±0.05	74.5±0.02	60.8±0.13
MEST _{1x}	51.47±0.1*	43.56±0.04*	75.22±0.57	58.85±1.08	51.58±0.15	43.28±0.15	78.47±0.14*	65.27±0.05	74.65±0.1	61.83±0.17
CHT _{1x} (WS, β = 1)	51.85±0.05*	44.92±0.02*	78.14±0.08*	65.31±0.14*	53.52±0.07*	47.1±0.1*	79.2±0.16*	67.51±0.1*	75.17±0.02*	63.7±0.07*
FC _{2x}	50.82±0.05	43.24±0.03	76.76±0.21	63.11±0.09	51.46±0.13	44.43±0.1	78.49±0.07	65.76±0.02	74.91±0.02	63.52±0.04
RigL _{2x}	51.5±0.11*	43.35±0.05*	74.89±0.44	58.41±0.44	52.12±0.09*	43.53±0.01	78.3±0.14	64.8±0.03	74.66±0.07	61.7±0.06
MEST _{2x}	51.36±0.08*	43.67±0.05*	75.54±0.01	60.49±0.02	51.59±0.07*	43.25±0.03	78.45±0.13	64.98±0.16	74.76±0.01	62.0±0.03
CHT _{1x} (WS, β = 1)	51.56±0.21*	43.84±0.29*	77.74±0.13*	65.44±0.06*	53.62±0.14*	47.27±0.06*	79.25±0.1*	67.37±0.03*	75.1±0.09*	63.43±0.18





Yingtao Zhang

EPITOPOLOGICAL LEARNING AND CANNISTRACI- HEBB NETWORK SHAPE INTELLIGENCE BRAIN- INSPIRED THEORY FOR ULTRA-SPARSE ADVANTAGE IN DEEP LEARNING

**Yingtao Zhang^{1,2,3}, Jialin Zhao^{1,2,3}, Wenjing Wu^{1,2,3}, Alessandro Muscoloni^{1,2,4},
& Carlo Vittorio Cannistraci^{1,2,3,4} ***

¹Center for Complex Network Intelligence (CCNI)

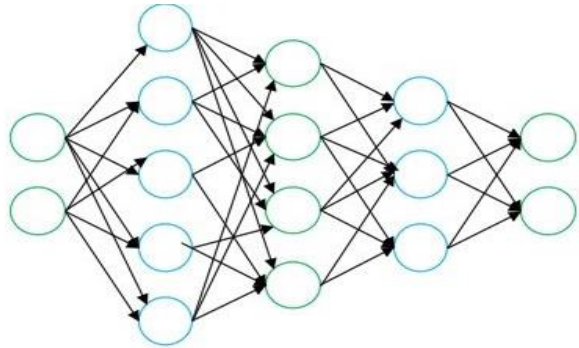
²Tsinghua Laboratory of Brain and Intelligence (THBI)

³Department of Computer Science, ⁴Department of Biomedical Engineering
Tsinghua University, Beijing, China.

ICLR2024 evaluation: avg. score 7.33, ranks 326/2261 accepted (in the top 15%)

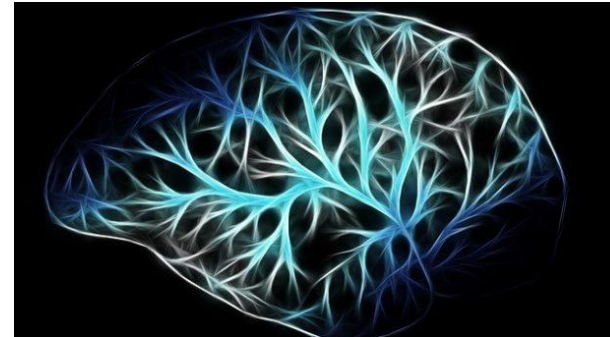
Crisis: I was a Master student in 2002

Artificial Neural Network (ANN)



Vs.

Brain Connectivity

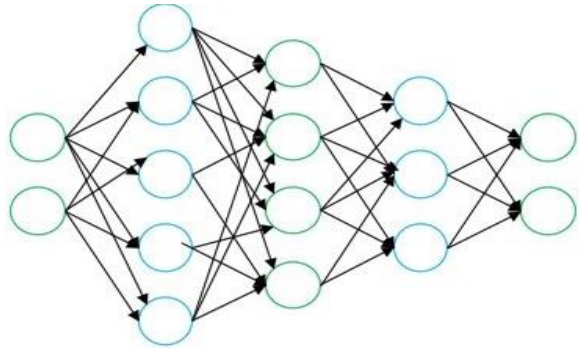


Crisis: Why is brain connectivity sparse?

- 1. What is the computational advantage of connectivity sparsity in brain biology?*
- 2. How to make profit of brain-inspired connectivity sparsity in ANN?*

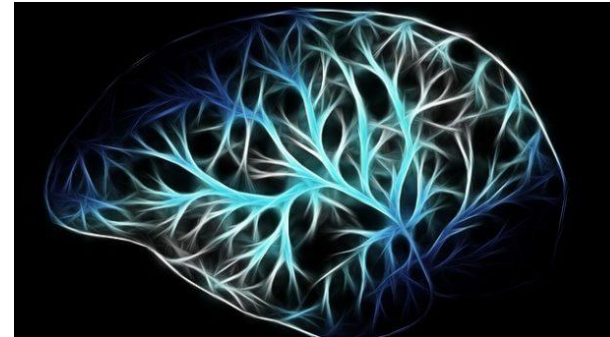
Crisis: I was a Master student in 2002

Artificial Neural Network (ANN)



Vs.

Brain Connectivity

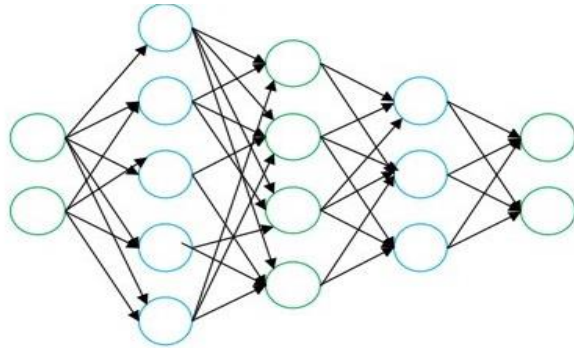


Crisis: Why is brain connectivity sparse?

***A 20 years long research path to address
a philosophical question***

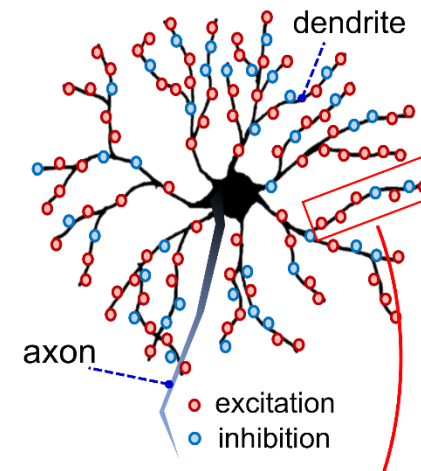
Question2: Network Morphology

Artificial Neural Network (ANN)



Vs.

Brain Morphology



Crisis: Why is brain connectivity sparse (topology)?

*Crisis: What is the contribution of **morphology**?*

OUTLINE of the talk

1. Prediction of connectivity in sparse network structures
2. Dynamic sparse training in deep learning
3. Neuromorphic computing

preprints.org > [computer science and mathematics](#) > [artificial intelligence and machine learning](#) > doi: 10.20944/preprints2

Preprint Article Version 1 Preserved in Portico This version is not peer-reviewed

Neuromorphic Dendritic Computation with Silent Synapses for Visual Motion Perception

 Eunhye Baek ^{*},  Sen Song,  Zhao Rong,  Luping Shi ^{*},  Carlo Vittorio Cannistraci ^{*}  ID

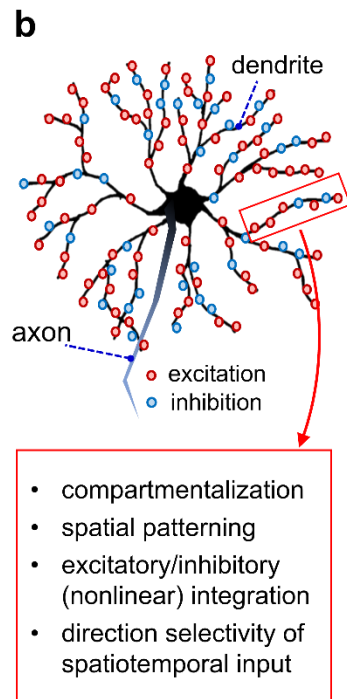
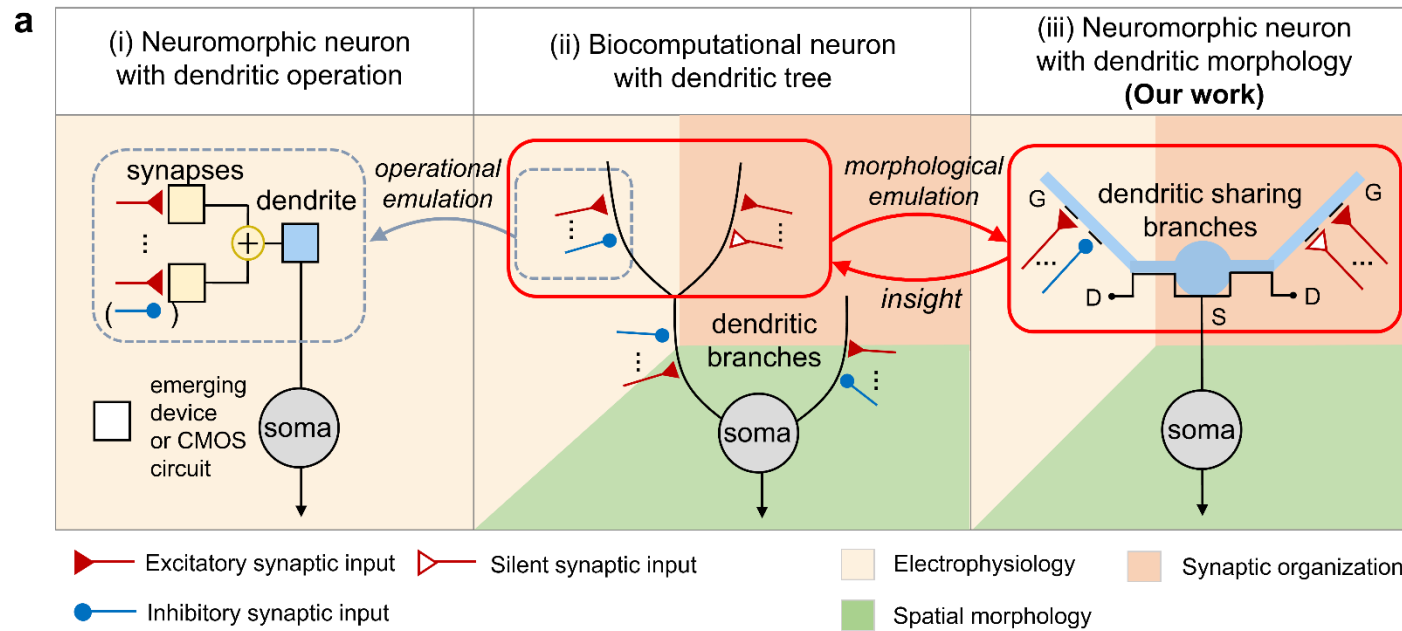
Version 1 : Received: 5 June 2023 / Approved: 6 June 2023 / Online: 6 June 2023 (10:04:05 CEST)

How to cite: Baek, E.; Song, S.; Rong, Z.; Shi, L.; Cannistraci, C.V. Neuromorphic Dendritic Computation with Silent Synapses for Visual Motion Perception. *Preprints* **2023**, 2023060438. <https://doi.org/10.20944/preprints202306.0438.v1> [Copy](#)

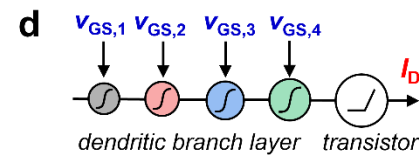
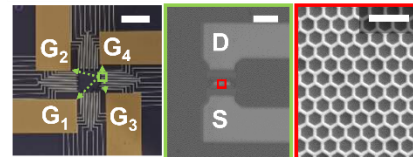
Abstract

Most neuromorphic technologies use a point-neuron model, missing the spatiotemporal nature of neuronal computation performed in dendrites. Dendritic morphology and synaptic organization are structurally tailored for spatiotemporal information processing, enabling various computations like visual perception. Here, we report on a neuromorphic computational model termed ‘dendristor’, which integrates functional synaptic organization with dendritic tree-like morphology computation. The dendristor presents bioplausible nonlinear integration of excitatory and inhibitory synaptic inputs with silent synapses and diverse spatial distribution dependency. We show that the dendristor can emulate direction selectivity, which is the feature to react robustly to a preferred signal direction on the dendrite. We discover that silent synapses can remarkably enhance direction selectivity, turning out to be a crucial player in dendritic computation processing. Finally, we develop neuromorphic dendritic neural circuits that can emulate a cognitive function such as motion perception in the retina. Using dendritic morphology, we achieve visual perception of motion in 3D space by various mapping of spatial information on different dendritic branches. This neuromorphic dendritic computation innovates beyond current neuromorphic computation and provides solutions to explore new skylines in artificial intelligence, neurocomputation, and brain-inspired computing.

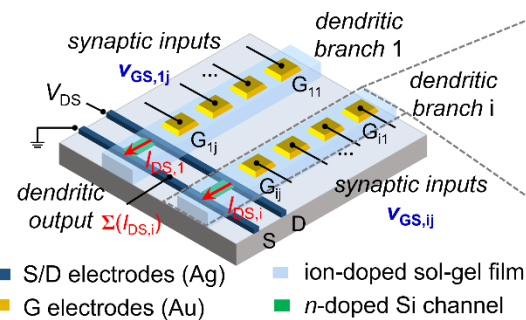
Nature Electronics 2024 Accepted



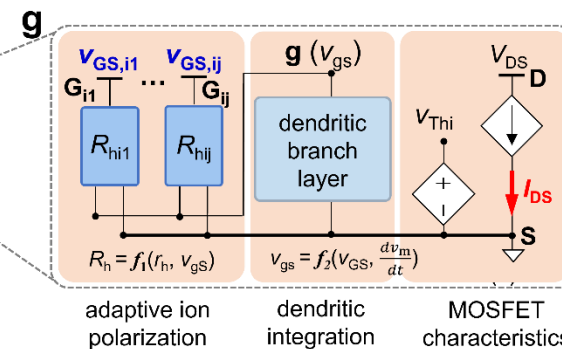
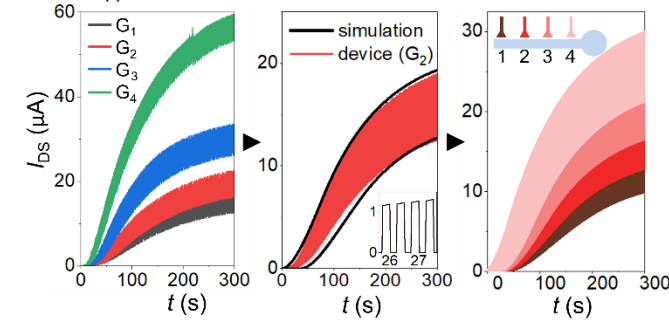
c Single dendritic branch - device



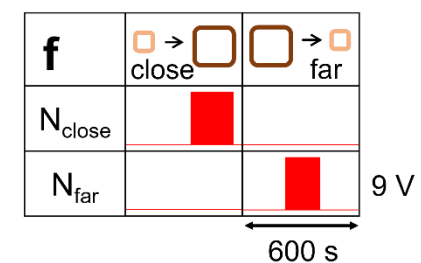
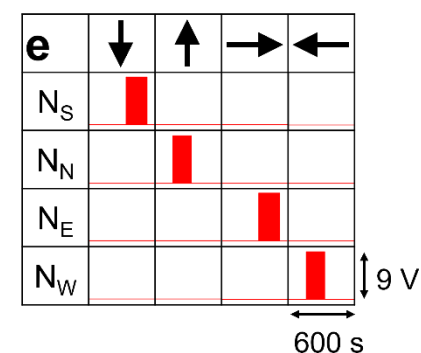
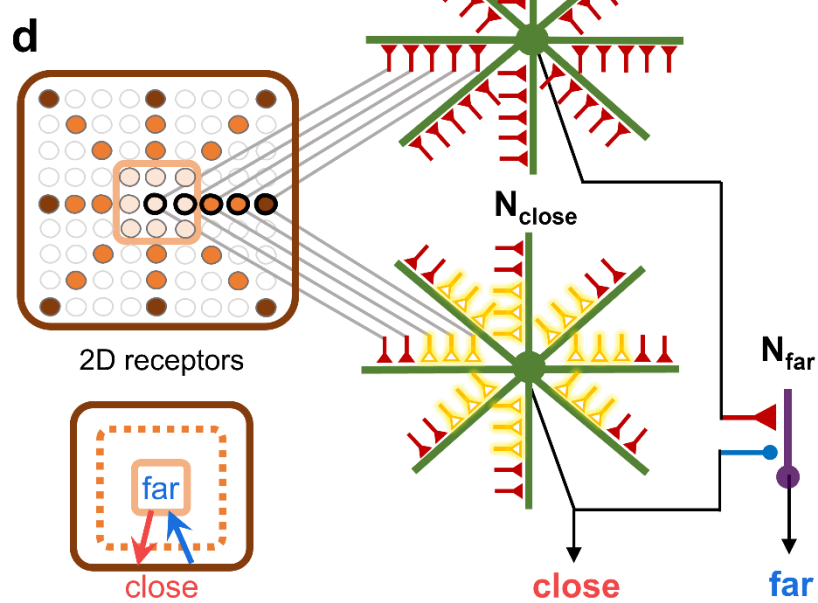
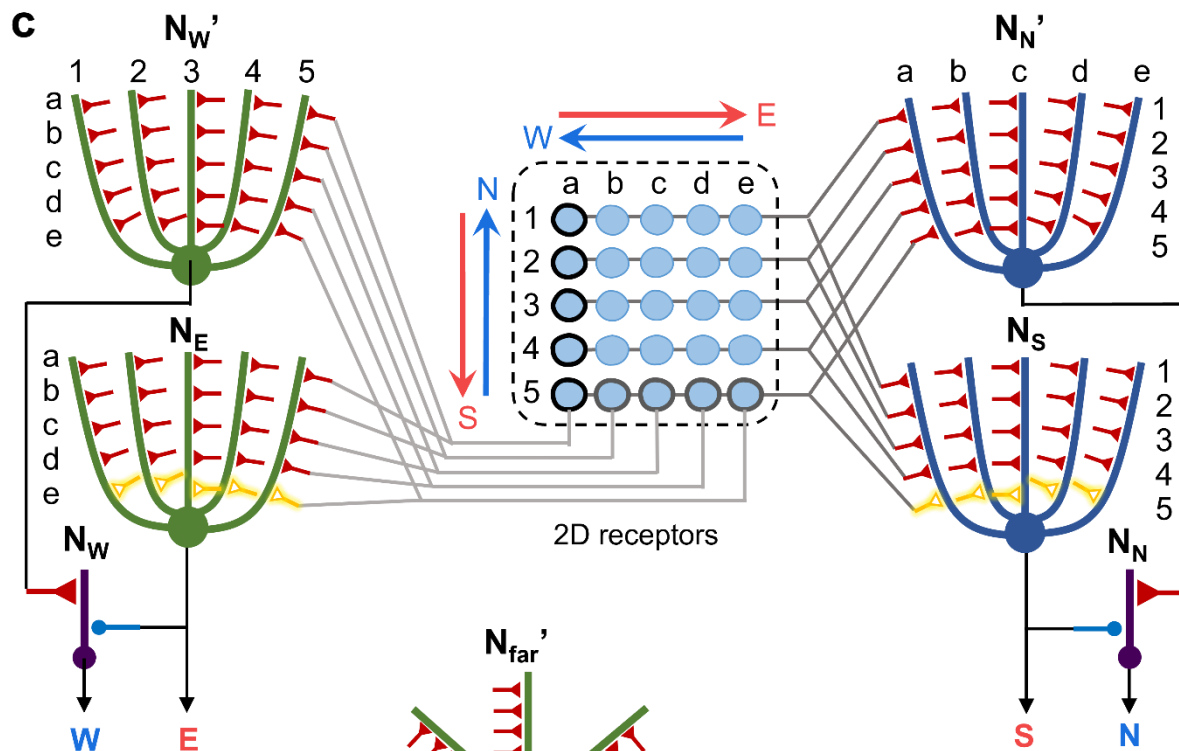
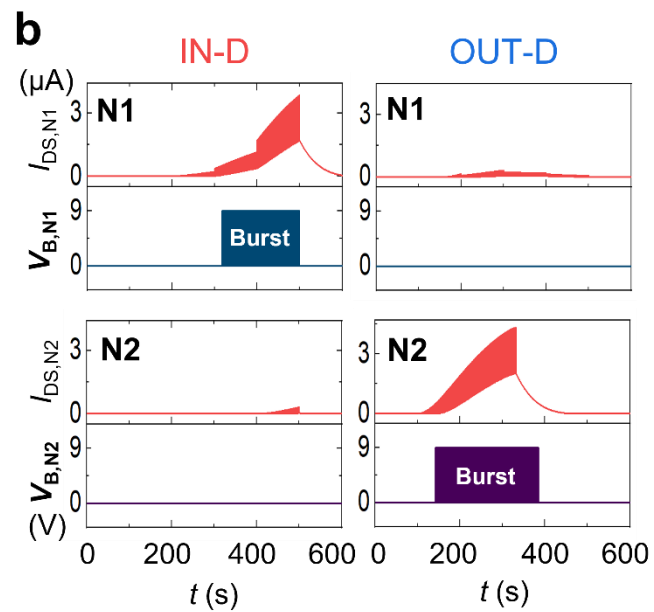
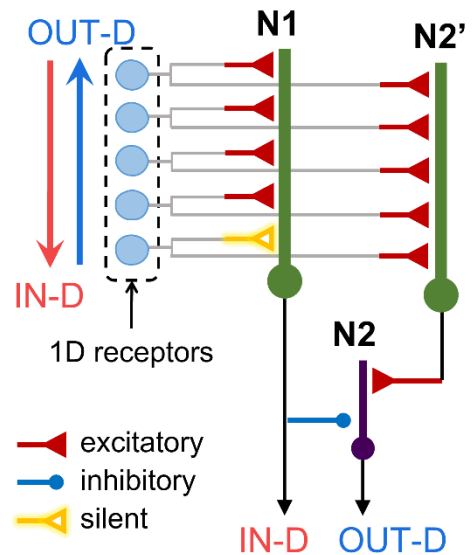
e Multiple dendritic branches - simulation

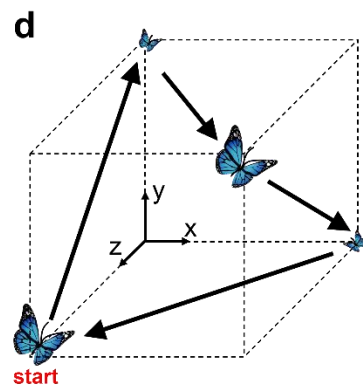
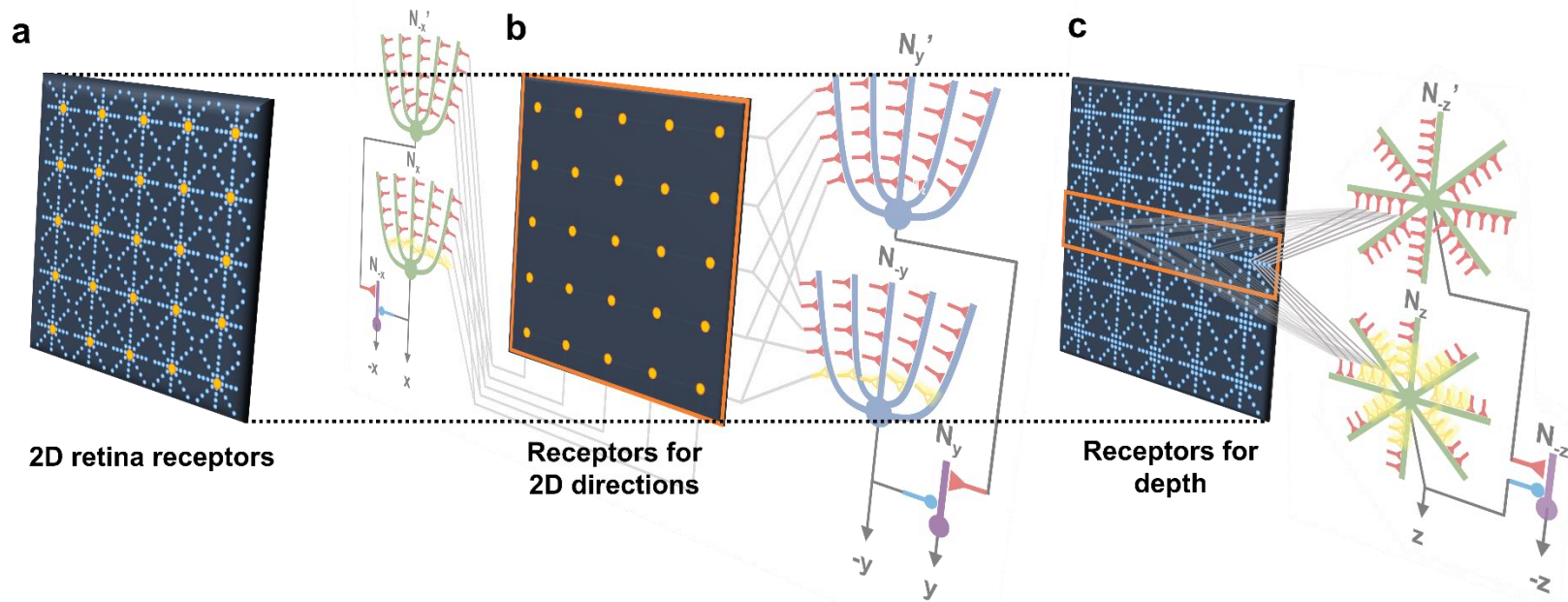


f (i) device (ii) standard model (iii) simulation

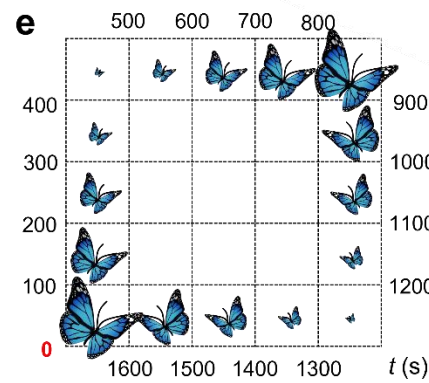


a Direction selective neuromorphic neural circuit (NNC)

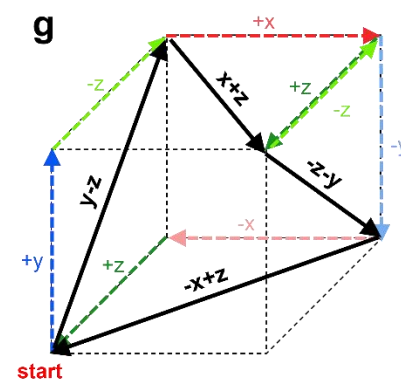




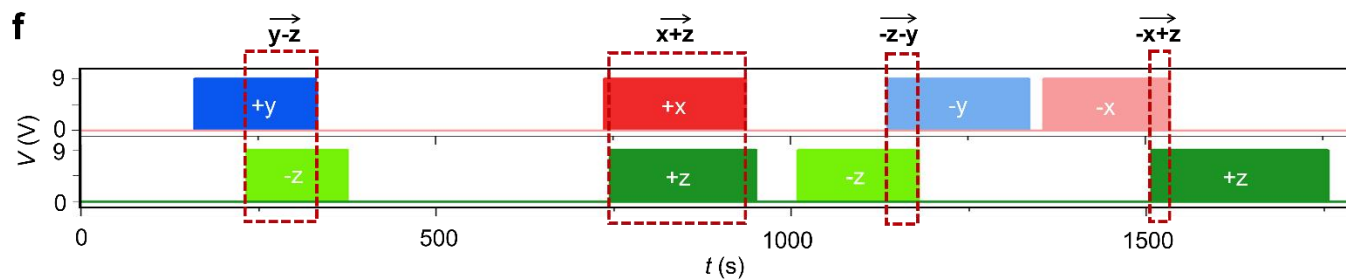
Real movement in 3D space

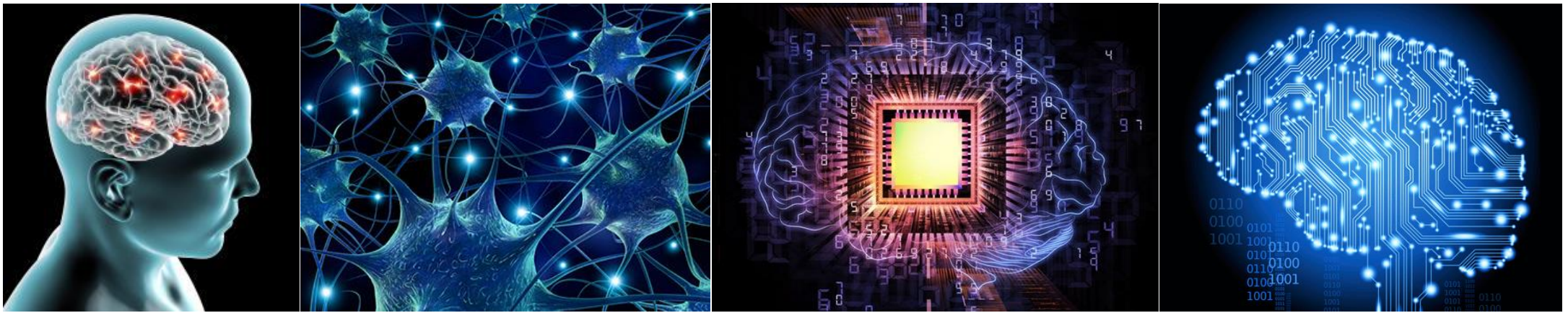


Projection on 2D retina receptors



Reconstruction in 3D space





Neuromorphic engineering for modelling dendritic computation with silent synapses

Tsinghua Univ,
China



Prof. C. V. Cannistraci

**Bioengineering
modeling**

Tsinghua Univ,
China



Prof. S. Song

**Bioengineering
modeling**

Tsinghua Univ,
China



Dr. E. Baek

**Neuromorphic
modeling**

Tsinghua Univ,
China



Prof. Z. Rong

**Neuromorphic
modeling**

Tsinghua Univ,
China



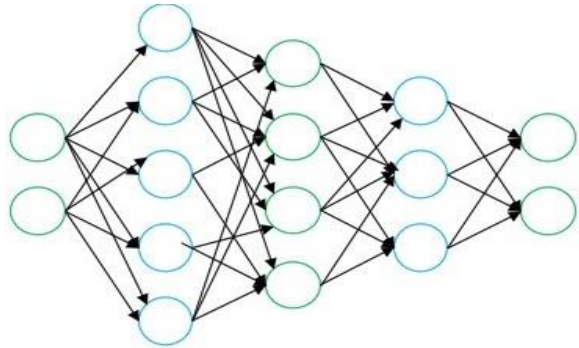
Prof. L. Shi

**Neuromorphic
modeling**



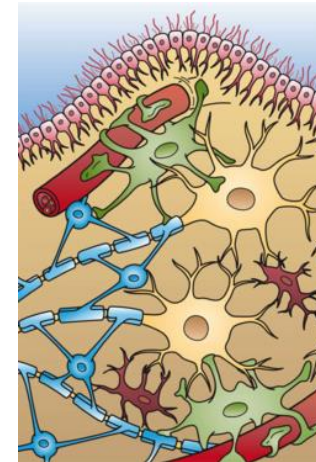
Crisis: I was a Master student in 2002

Artificial Neural Network (ANN)



Vs.

Brain cell coupling



Crisis: Why is brain connectivity sparse (topology)?

Crisis: What is the contribution of morphology?

Crisis: What is the contribution of **neuro-glia coupling**?

Scientific Institutions



San Raffaele
Scientific Institute



center for
systems biology
dresden



- Lipotype (Germany)
- Politecnico di Torino and Milano (Italy)
- Italian Interpolytechnic School of Doctorate (SIPD, Italy)
- San Raffaele Scientific Institute, Hospital and University (Italy)
- King Abdullah University of Science and Technology (KAUST, Saudi Arabia)
- University of California San Diego/ Ideker Lab (USA)
- ISMB/ECCB generously provided me (International)
- Italian National Research Council (CNR) / Bioengineering (It)
- Technical University Dresden (Germany)
- Klaus Tschira Foundation (Germany)
- FANTOM Consortium and RIKEN institute (Japan)



CENTRO NEUROLESI
BONINO PULEJO
IRCCS MESSINA



清华大学脑与智能实验室
Tsinghua Laboratory of Brain and Intelligence



Politecnico
di Torino



清华大学
Tsinghua University



TECHNISCHE
UNIVERSITÄT
DRESDEN



Carlo Vittorio Cannistraci

*Center for Complex Network
Intelligence*

EMAIL: kalokagathos.agon@gmail.com

Thanks!



清华大学
Tsinghua University



清华大学脑与智能实验室
Tsinghua Laboratory of Brain and Intelligence