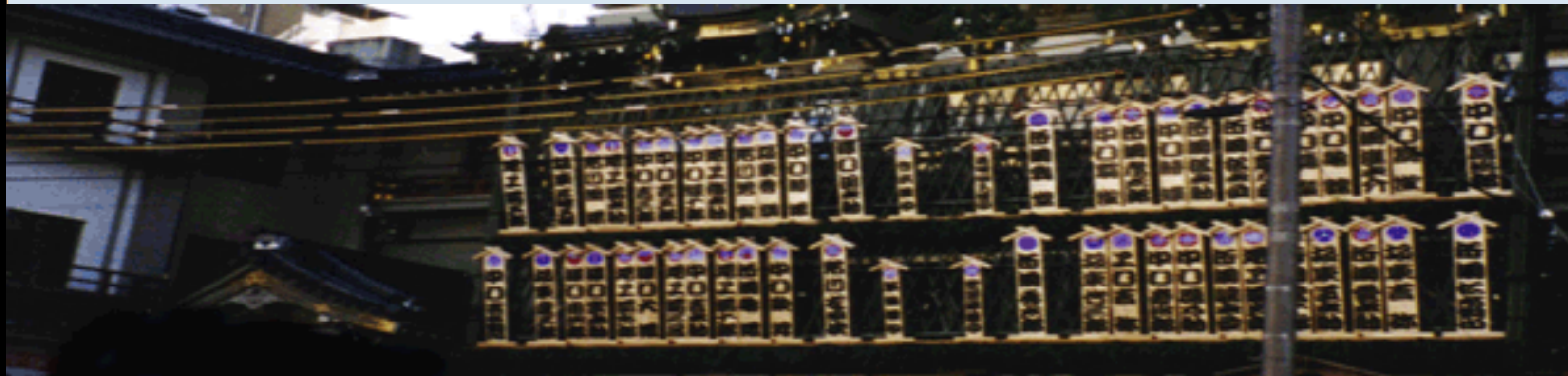
redundancy, control and collective computation



in network dynamics

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casci CNetS Cognitive Science Program FUNDAÇÃO CALOUSTE GULBENKIAN Instituto Gulbenkian de Ciência

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acknowledgements

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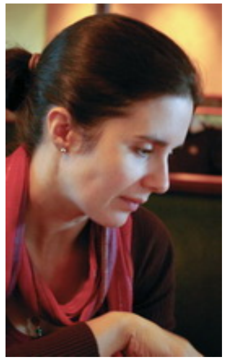

Anália Lourenço


Tiago Simas


Artemy Kolchinsky


Santosh Manicka

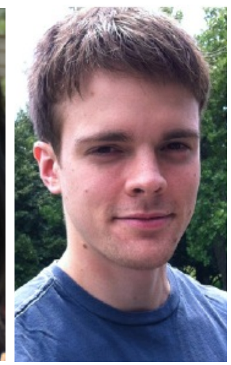

Alexander Gates


Jason Yoder


Ian Wood


Rion Brattig Correia


Yizhi Jing


Thomas Parmer

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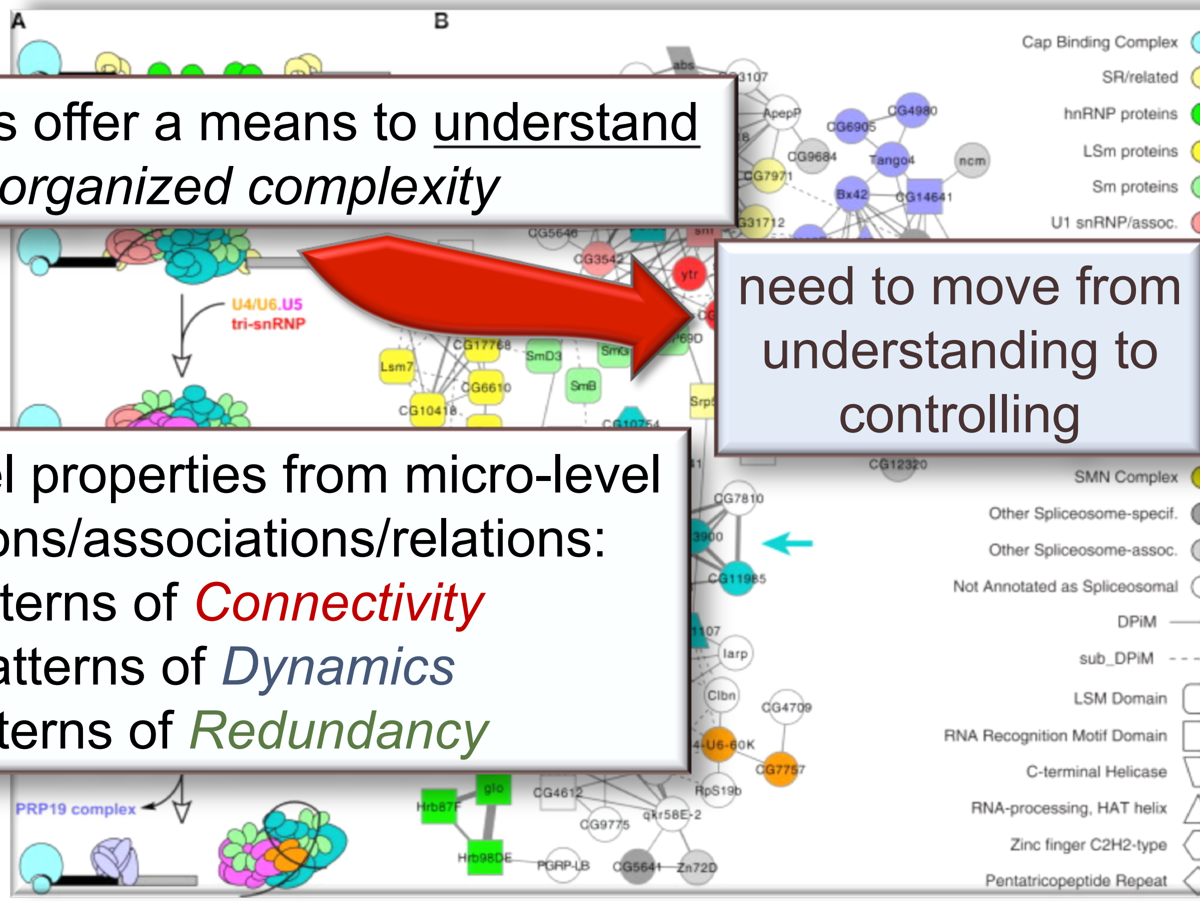
large-scale *drosophila protein interaction Map* (DPiM)

Guruharsha et al [2011]. “A Protein Complex Network of Drosophila melanogaster.” *Cell*.**147**(3):690-703.



Networks offer a means to <u>understand</u> *organized complexity*

need to move from understanding to controlling

Macro-level properties from micro-level interactions/associations/relations:
Patterns of *Connectivity*
Patterns of *Dynamics*
Patterns of *Redundancy*

Modularity of the spliceosome subnetwork: 12 well-connected clusters representing interaction of snRNPs with pre-mRNA and other proteins in the process of splicing introns.

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PATTERNS OF REDUNDANCY IN DYNAMICS

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the drosophila segment polarity network

an automata network model built from qualitative data

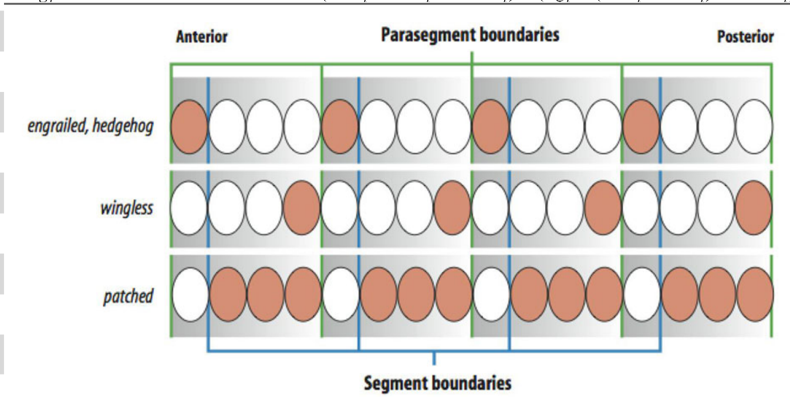
Based on the ODE model of von Dassow et al. (2000), consists of 4-cell parasegments, each cell with 15 interacting genes and proteins.

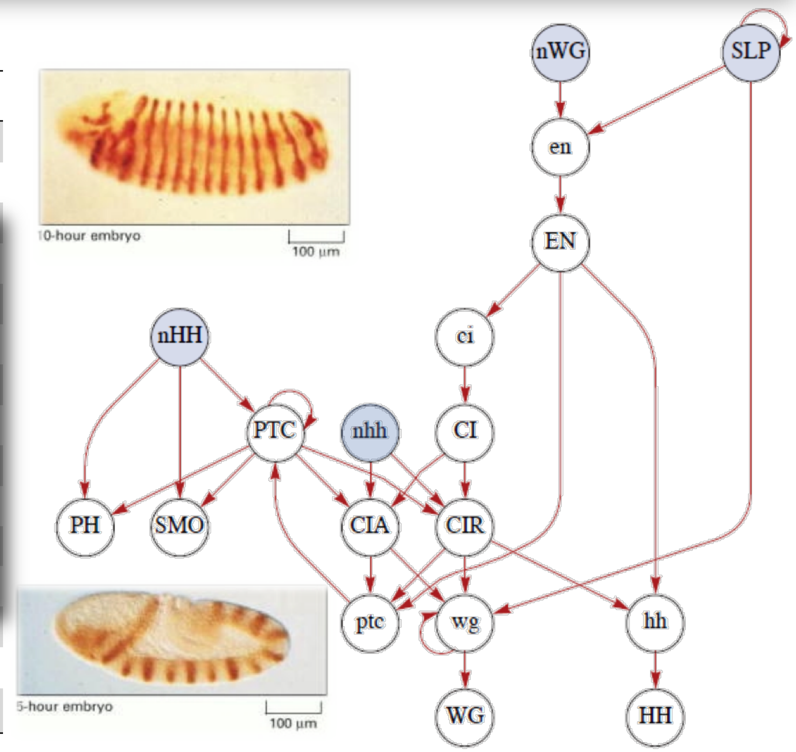
2^{60} network configurations

Reproduces wild-type and mutant gene expression patterns in development of fruit fly

- 2 intercellular inputs: **nhh** (*hedgehog*), **nWG** (*wingless*)
- 1 intracellular input: **SLP** (*sloppy paired*)

Node	*State – TransitionFunction*
SLP_i^{t+1}	$\leftarrow 0$ if $i=1 \vee i=2$; 1 if $i=3 \vee i=4$;
wg_i^{t+1}	$\leftarrow (CIA_i^t \wedge SLP_i^t \wedge \neg CIR_i^t) \vee (wg_i^t \wedge (CIA_i^t \vee SLP_i^t) \wedge \neg CIR_i^t)$
CI_i^{t+1}	$\leftarrow ci_i^t$
CIA_i^{t+1}	$\leftarrow CI_i^t \wedge (\neg PTC_i^t \vee hh_{i-1}^t \vee hh_{i+1}^t \vee HH_{i-1}^t \vee HH_{i+1}^t)$
CIR_i^{t+1}	$\leftarrow CI_i^t \wedge PTC_i^t \wedge \neg hh_{i-1}^t \wedge \neg hh_{i+1}^t \wedge \neg HH_{i-1}^t \wedge \neg HH_{i+1}^t$





Albert & Othmer [2003]. *J. Theor. Bio.* **223**: 1-18.

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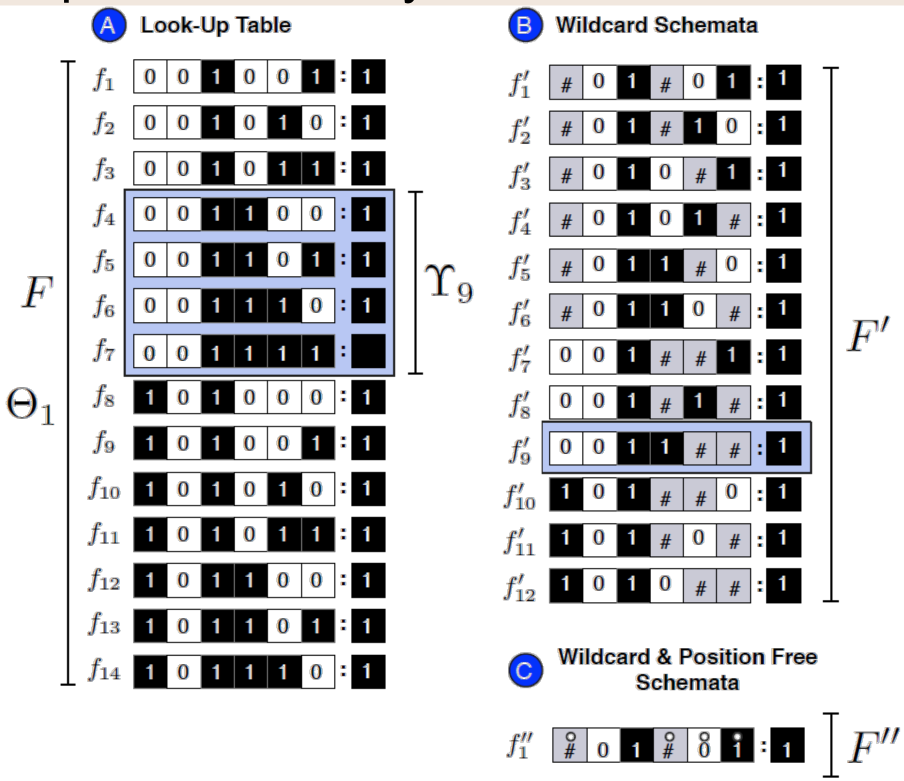
quantifying micro-level canalization

input redundancy, effective connectivity and input symmetry



$$k(x) = 6$$

$$k_r(x) = \frac{\sum_{f_\alpha \in F} \max_{\theta | f_\alpha \in \Theta_\theta} \left(n_\theta^{\#}\right)}{2^k}$$

$$k_e(x) = k(x) - k_r(x)$$

$$k_s(x) = \frac{\sum_{f_\alpha \in F} \min_{\theta | f_\alpha \in \Theta_\theta} \left|n_\theta^{o}\right|}{2^k}$$

- Measuring two forms of *canalization*
  - $K_r = 2$
  - $K_e = 6 - 2 = 4$
  - $K_s = 4$

Prime Implicants (Quine-McCluskey) plus **group invariance**



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Marques-Pita & Rocha, [2013]. *PLoS ONE*, **8**(3): e55946.

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per-node schema redescription

In biological Boolean network models

- extracting micro-level canalization
  - drosophila segment polarity genes network

node	inhibition	expression	k	k_e	k_r	k_s	k^*_r	k^*_s
wg	SLP, wg, CIA, CIR : wg — $f''_{2:1}$, $f''_{2:2}$	SLP, wg, CIA, CIR : wg — $f''_{2:3}$	4	1.75	2.25	2.25	0.56	0.56
PTC	ptc, PTC, HH_{i-1}, HH_{i+1} : PTC — $f''_{9:1}$, $f''_{9:2}$	ptc, PTC, HH_{i-1}, HH_{i+1} : PTC — $f''_{9:3}$, $f''_{9:4}$	4	1.56	2.44	0.75	0.61	0.19
PH	PTC, HH_{i-1}, HH_{i+1} : PH — $f''_{10:1}$, $f''_{10:2}$	PTC, HH_{i-1}, HH_{i+1} : PH — $f''_{10:3}$	3	1.5	1.5	0.75	0.5	0.25
SMO	PTC, HH_{i-1}, HH_{i+1} : SMO — $f''_{11:1}$	PTC, HH_{i-1}, HH_{i+1} : SMO — $f''_{11:2}$, $f''_{11:3}$	3	1.25	1.75	1.5	0.58	0.5
ci	EN : ci — $f''_{12:1}$	EN : ci — $f''_{12:2}$	1	1	0	0	0	0
CI	ci : CI — $f''_{13:1}$	ci : CI — $f''_{13:2}$	1	1	0	0	0	0
CIA	PTC, CI, hh_{i-1}, hh_{i+1}, HH_{i-1}, HH_{i+1} : CIA — $f''_{14:1}$, $f''_{14:2}$	PTC, CI, hh_{i-1}, hh_{i+1}, HH_{i-1}, HH_{i+1} : CIA — $f''_{14:3}$, $f''_{14:4}$	6	1.55	4.45	1.875	0.74	0.32
CIR	PTC, CI, hh_{i-1}, hh_{i+1}, HH_{i-1}, HH_{i+1} : CIR — $f''_{15:1}$, $f''_{15:2}$	PTC, CI, hh_{i-1}, hh_{i+1}, HH_{i-1}, HH_{i+1} : CIR — $f''_{15:3}$	6	1.08	4.92	5.25	0.82	0.88

per-node schema redescription

In biological Boolean network models

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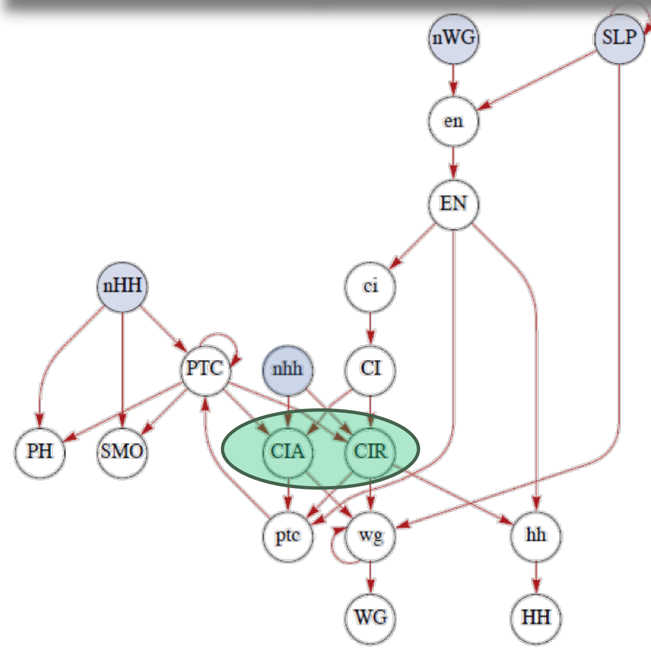
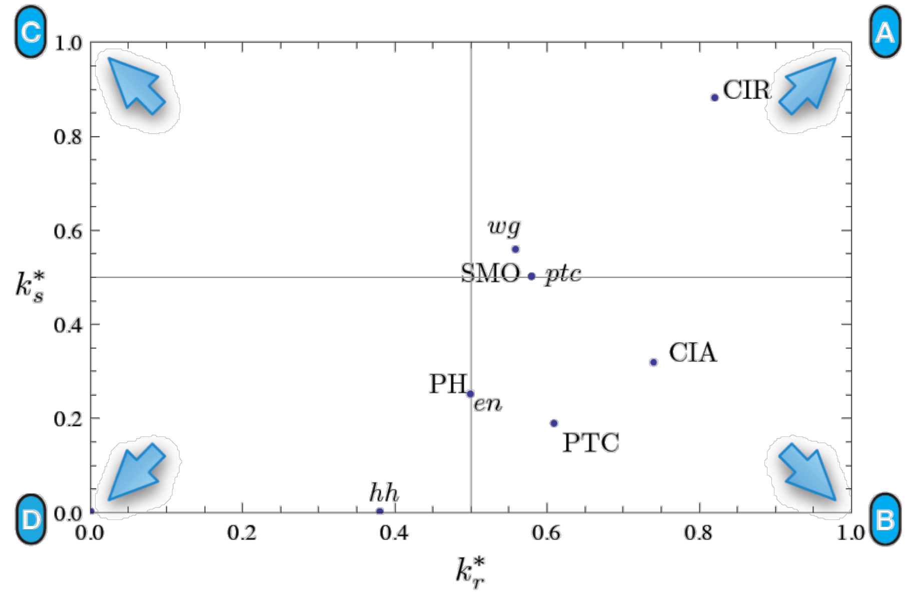
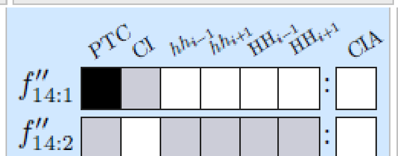
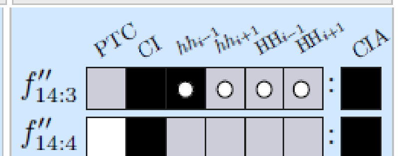
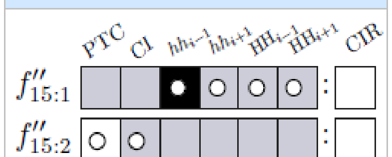
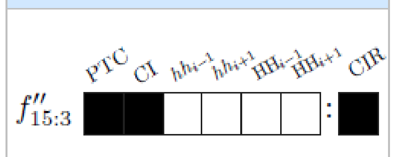
- extracting micro-level canalization
  - drosophila segment polarity genes network





node	inhibition	expression	k	k_e	k_r	k_s	k_r^*	k_s^*
CIA			6	1.55	4.45	1.875	0.74	0.32
CIR			6	1.08	4.92	5.25	0.82	0.88

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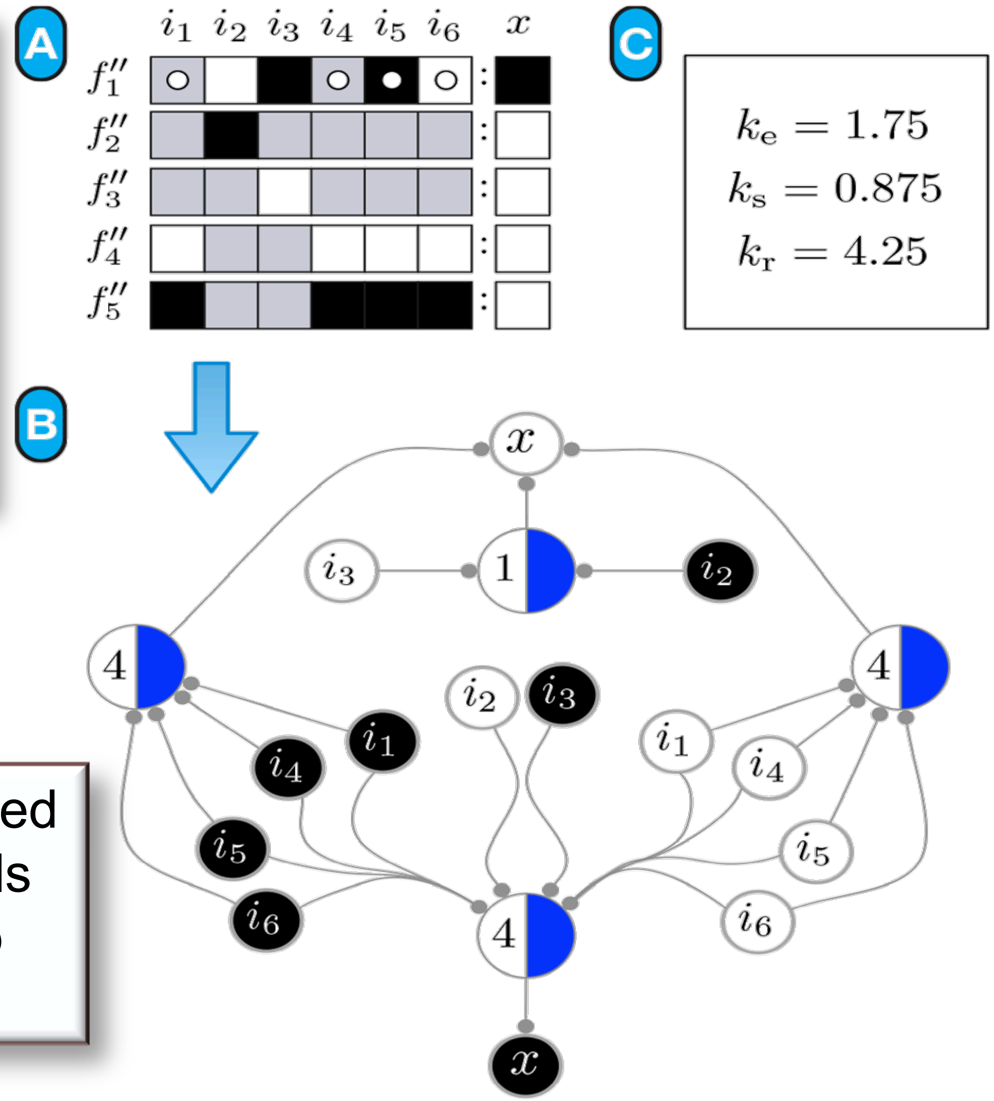
canalization map as minimal control

two-symbol schemata as threshold networks

- understanding natural "computation"
  - How cells compute
  - minimal wiring (control) of **micro-level**



Each schema represented by conjunction of literals and symmetric group constraints

Marques-Pita & Rocha, [2013]. *PLoS ONE*, **8**(3): e55946.

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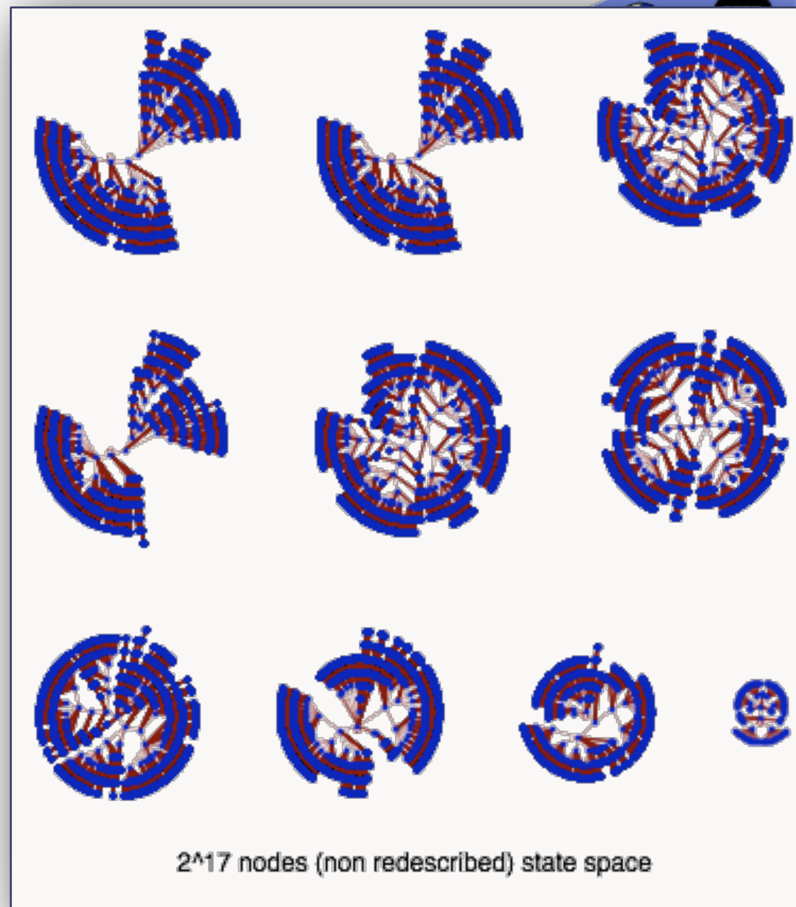
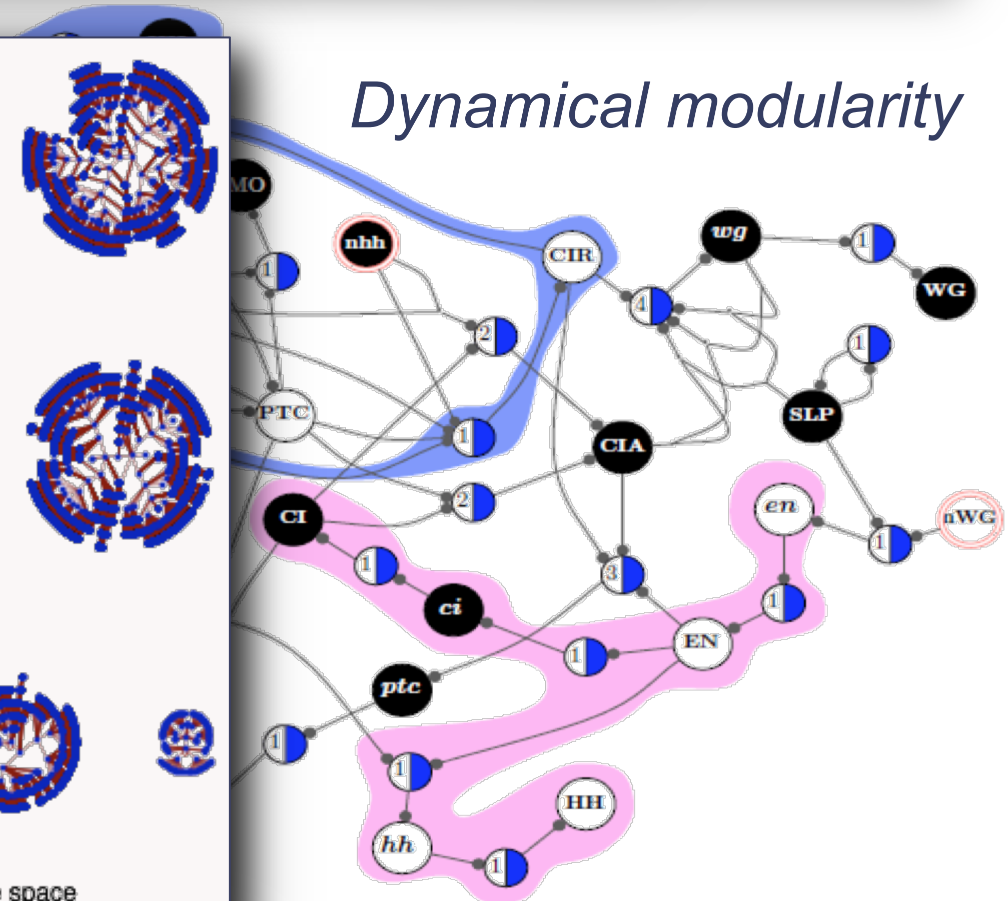
(macro-level) dynamics canalization map

from per-node schemata redescription

- Full dynamics (of single-cell model) captured by threshold network of 2*N+M nodes



Dynamical modularity



Marques-Pita & Rocha, [2013]. *PLoS ONE*, **8**(3): e55946.

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CONTROL FROM PATTERNS OF REDUNDANCY IN DYNAMICS

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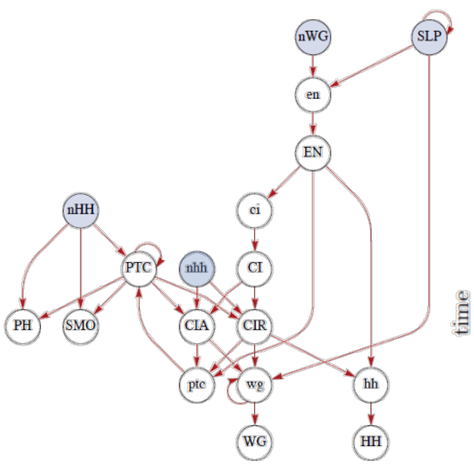
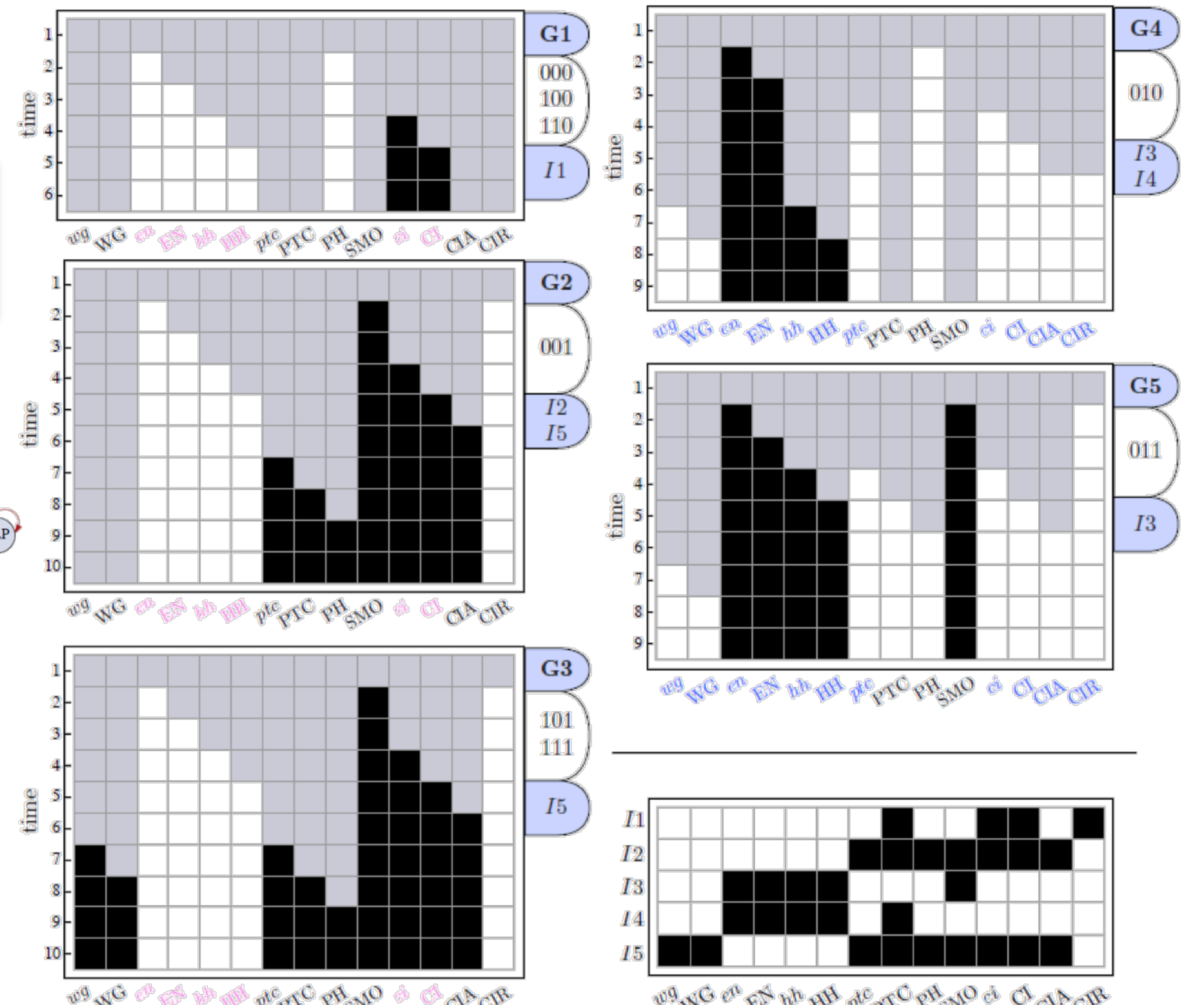
(macro-level) control

Dynamical unfolding from partial information

- inputs in drosophila segment polarity net: SLP, nWG, nhh

How much control certain nodes have on network dynamics.





Marques-Pita & Rocha, [2013]. *PLoS ONE*, **8**(3): e55946.

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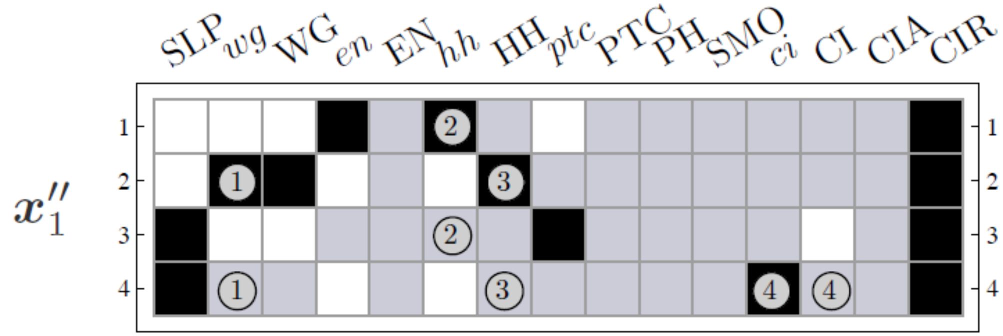
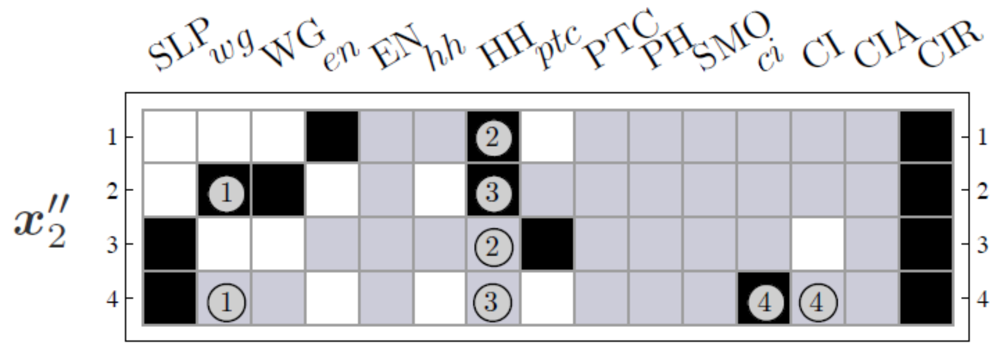
minimal conditions ("pre-patterns") for wild-type attractor





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Less than half of the nodes are needed to ensure convergence to **wt**, which is very **robust** and **larger** than previously thought.

But losing one essential input (enputs) leads to a "unspecific" attractor. In this case could go to wt, wt (ptc mutant) or no segmentation.

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Marques-Pita & Rocha, [2013]. *PLoS ONE*, **8**(3): e55946.

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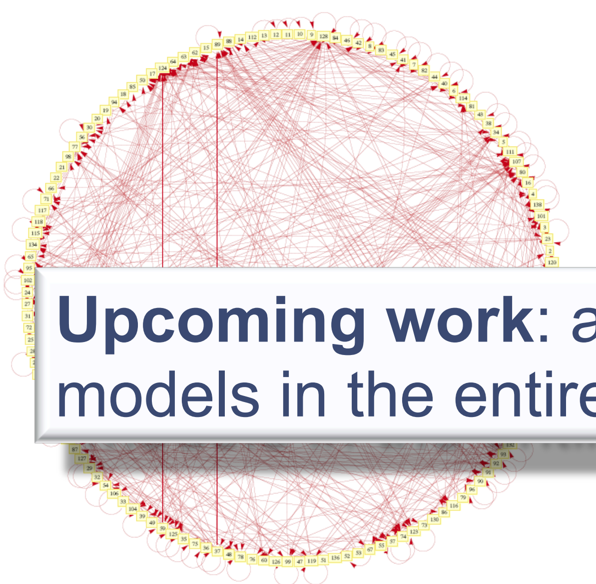
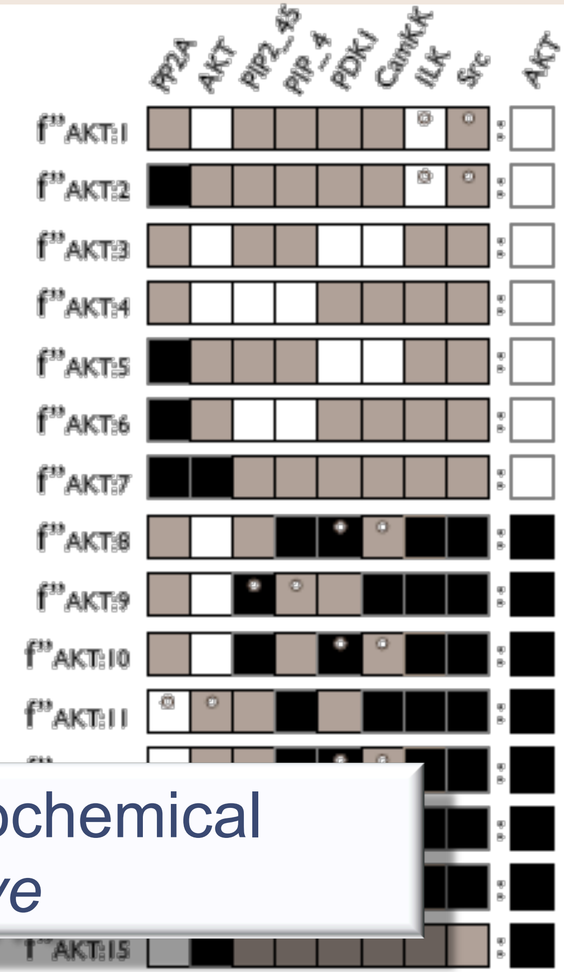
redundancy in intracellular signaling networks

canalization

- Activation of AKT in generic fibroblasts (130 node BN)
  - LUT of 2^8=256 entries redescribed by only 15 schemata
    - Large amount of **canalization**
  - Very few actual inputs need to be known to determine state-transition





Upcoming work: analysis of biochemical models in the entire *cell collective*

Helikar et al [2008]. PNAS **105**: 1913-8

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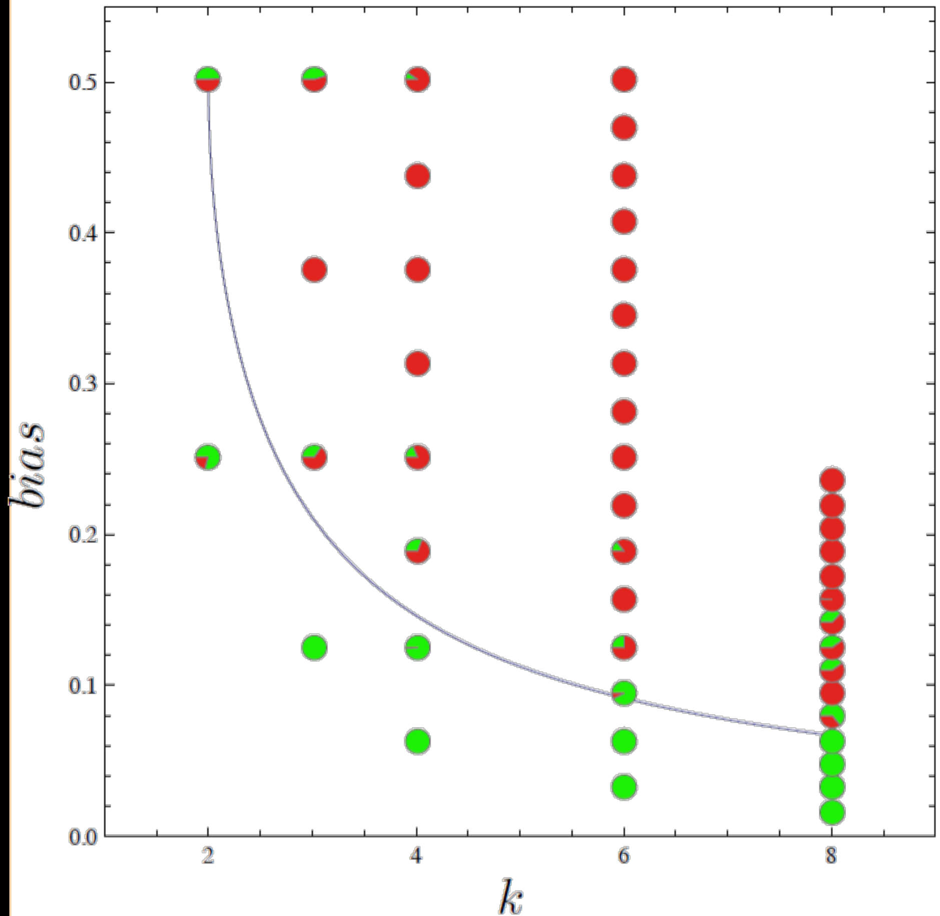
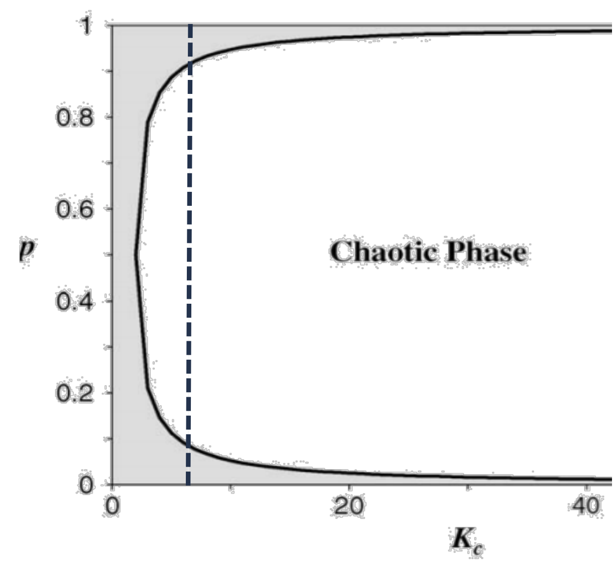
Current theory



$$p = \frac{1}{2}\left(1 - \sqrt{1 - \frac{2}{k}}\right)$$

Aldana, M. [2003]. *Physica D*. **185**: 45–66



Marques-Pita, Manicka, Teuscher & Rocha, [2014]. Submitted

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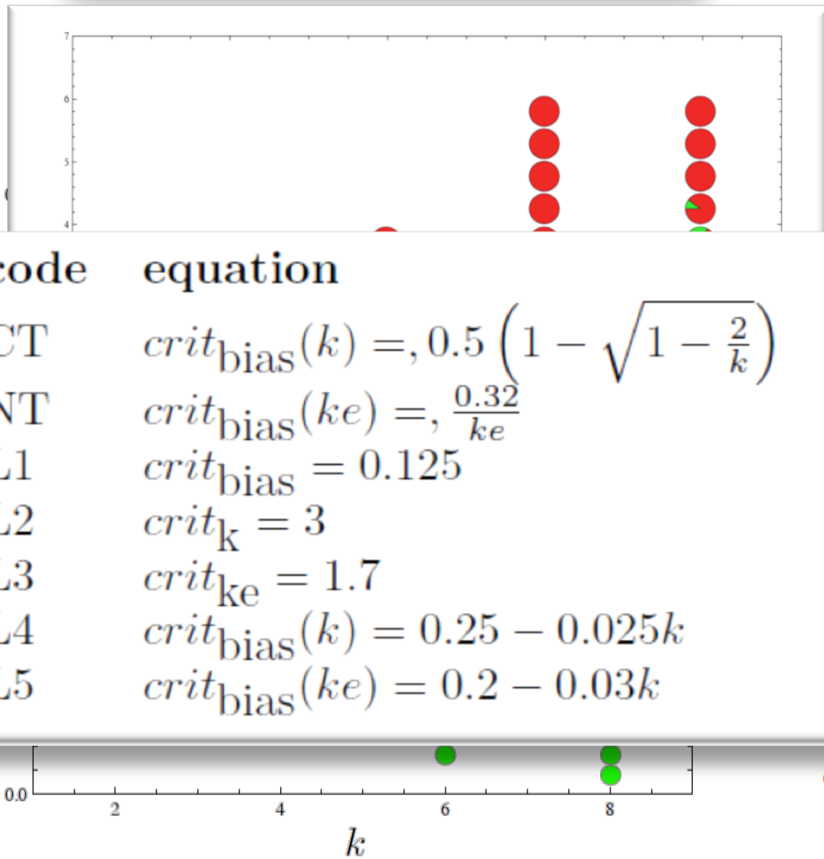
criticality in the presence of canalization

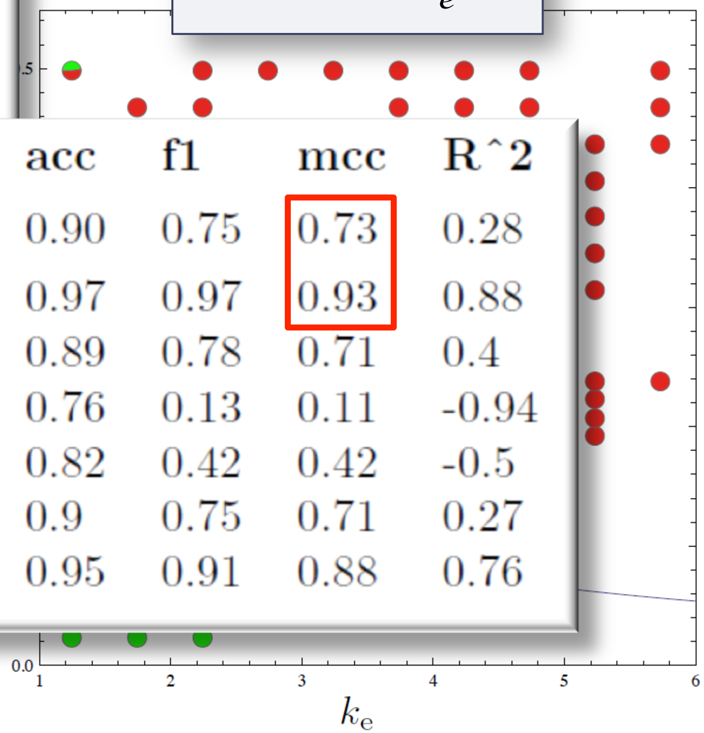
input redundancy, effective connectivity

$$k_r(x) = \frac{\sum_{f_\alpha \in F} \max_{\theta | f_\alpha \in \Theta_\theta} \left(n_\theta^{\#} \right)}{2^k}$$

$$k_e(x) = k(x) - k_r(x)$$

$$p_{crit} = \frac{0.32}{k_e}$$





code	equation	acc	f1	mcc	R^2
CT	$crit_{\text{bias}}(k) =, 0.5\left(1-\sqrt{1-\frac{2}{k}}\right)$	0.90	0.75	0.73	0.28
NT	$crit_{\text{bias}}(ke) =, \frac{0.32}{ke}$	0.97	0.97	0.93	0.88
L1	$crit_{\text{bias}} = 0.125$	0.89	0.78	0.71	0.4
L2	$crit_{\text{k}} = 3$	0.76	0.13	0.11	-0.94
L3	$crit_{\text{ke}} = 1.7$	0.82	0.42	0.42	-0.5
L4	$crit_{\text{bias}}(k) = 0.25 - 0.025k$	0.9	0.75	0.71	0.27
L5	$crit_{\text{bias}}(ke) = 0.2 - 0.03k$	0.95	0.91	0.88	0.76

Marques-Pita, Manicka, Teuscher & Rocha, [2014]. In preparation.

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from weighted graphs

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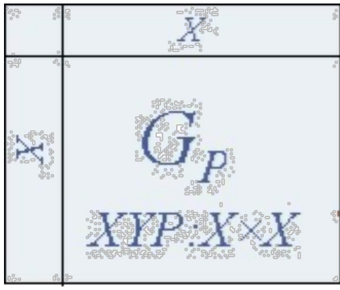
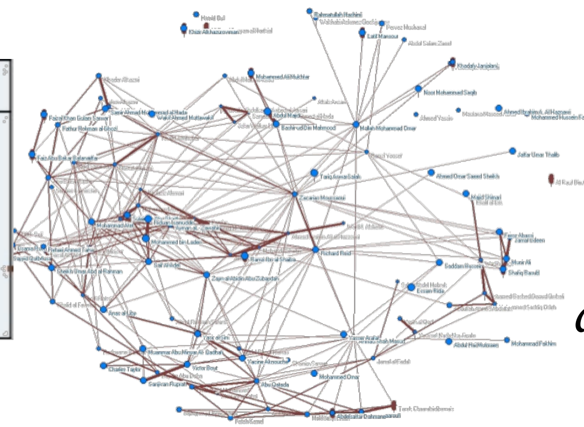
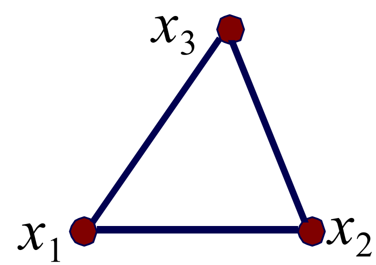
Proximity



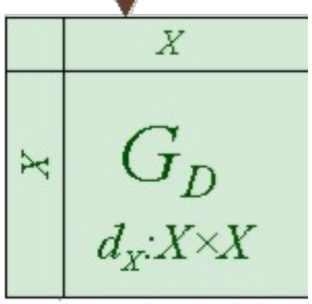




$$d(x_1, x_2) \quad d(x_1, x_3) + d(x_3, x_2)$$

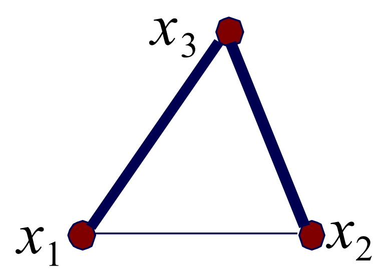
Metric

$$\varphi : d_X(x_i, x_j) = \frac{1}{XYP(x_i, x_j)} - 1$$



Distance

ϕ is a nonlinear **distance function:** nonnegative, symmetric, antireflexive ($d(x, x) = 0$)



$$d(x_1, x_2) > d(x_1, x_3) + d(x_3, x_2)$$

Semi-metric

Rocha & Bollen [2001] In: *SFI Series*. Segel & Cohen (Eds.), 305-334.
Rocha, L.M. [2002]. In: *Soft Computing Agents*: 137-163.
Rocha, L.M. et al [2005]. *IEEE Web Intelligence* (WI'05): 565-571.

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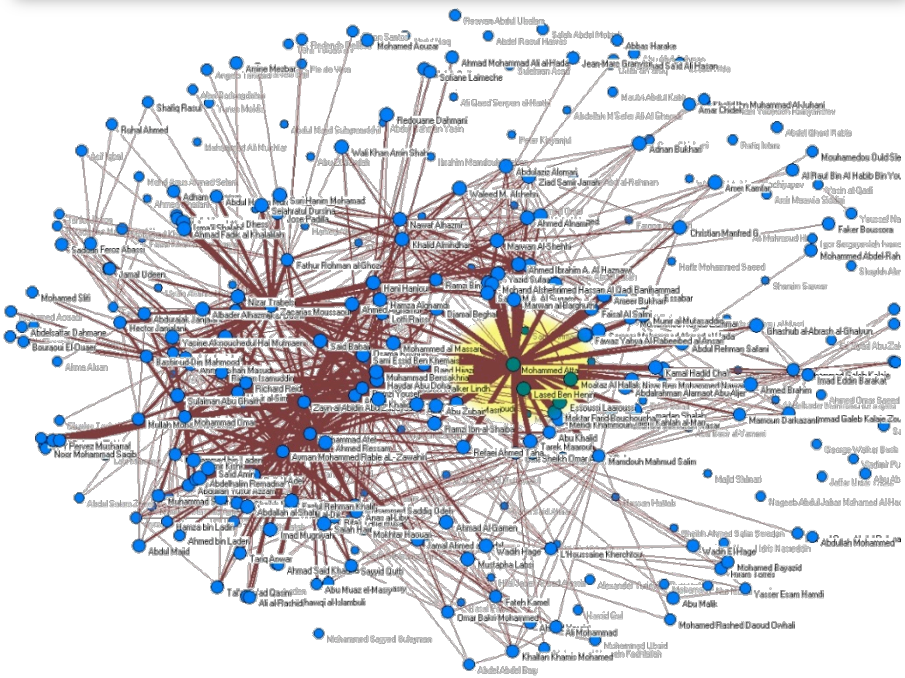
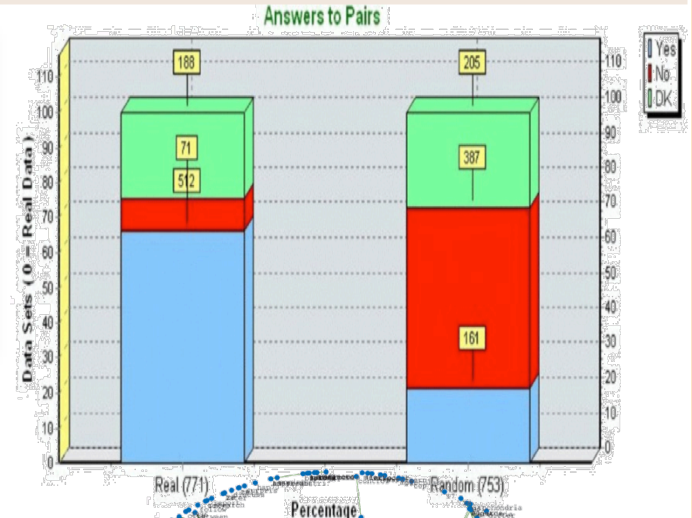
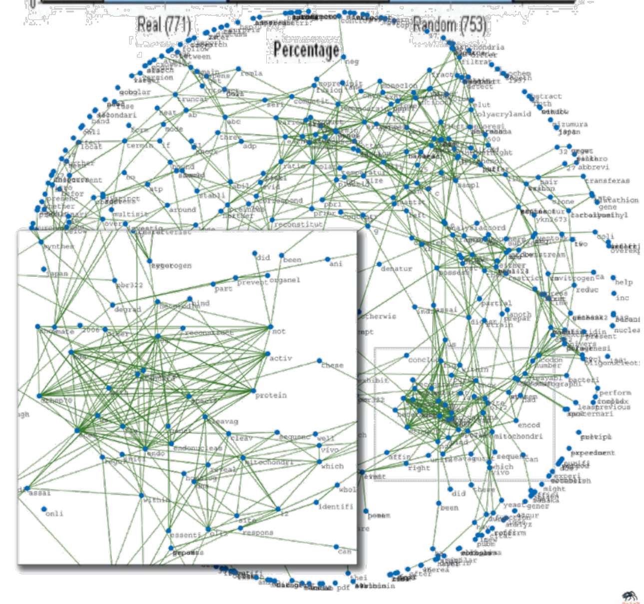
semi-metric edges

latent associations in data

- indirectly connected items
  - Higher change of future strength
- Applications
  - Recommender systems
  - Social biochemical networks







Rocha, L.M. et al [2005]. *IEEE Web Intelligence* (WI'05): 565-571.
Simas & Rocha [2012]. *IEEE Web Intelligence* (WI‘12). 175-179.
Abi-Haidar, A et al. [2008] *Genome Biology* **9**(Suppl 2):S11.

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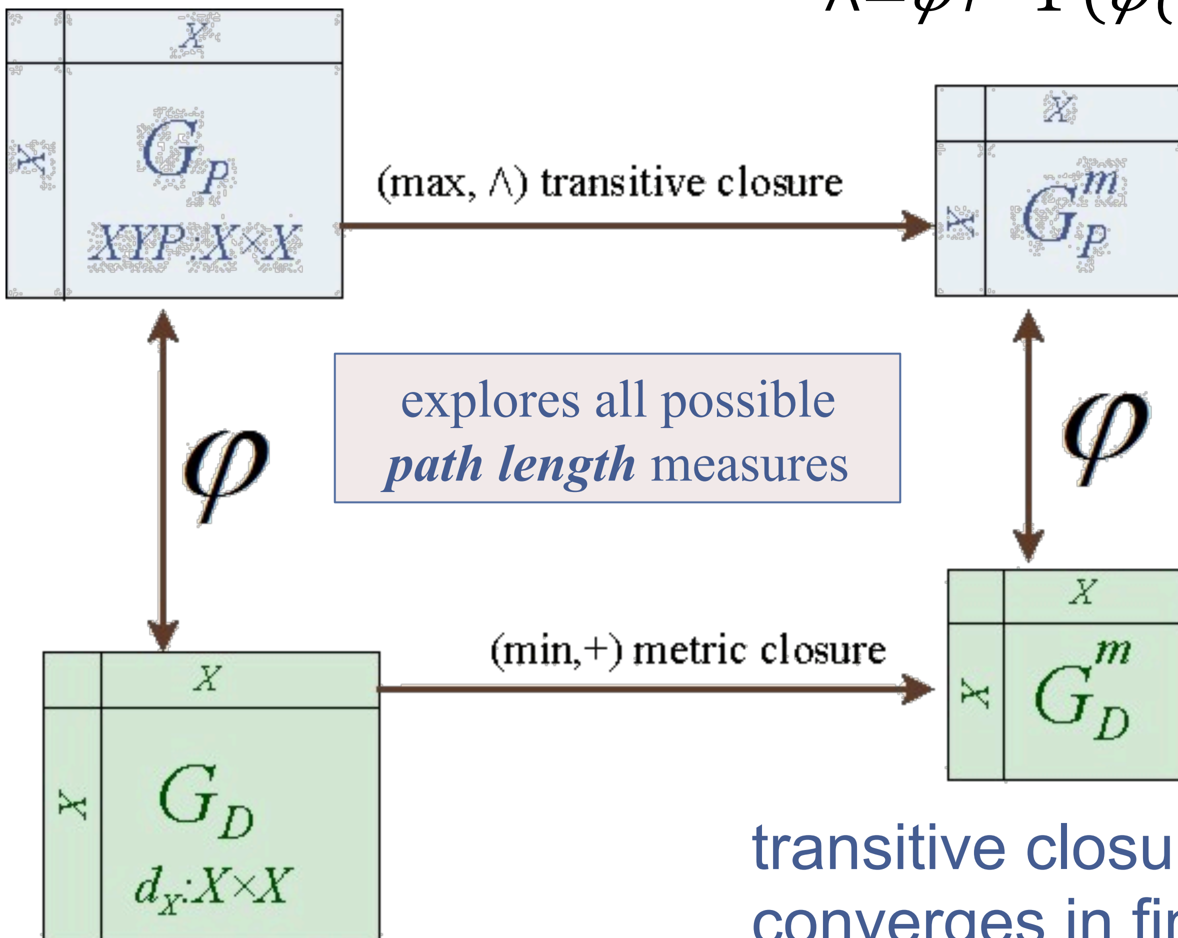
generalized distance closure with APSP (Dijkstra)

$$\wedge = \varphi^{-1}(\varphi(a)+\varphi(b))$$



Semi-metric distance graphs

transitive closure converges in finite time

Simas & Rocha [2014]. *Network Science*. In Press. arXiv:1312.2459

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ultra-metric closure ($\vee$=maximum)

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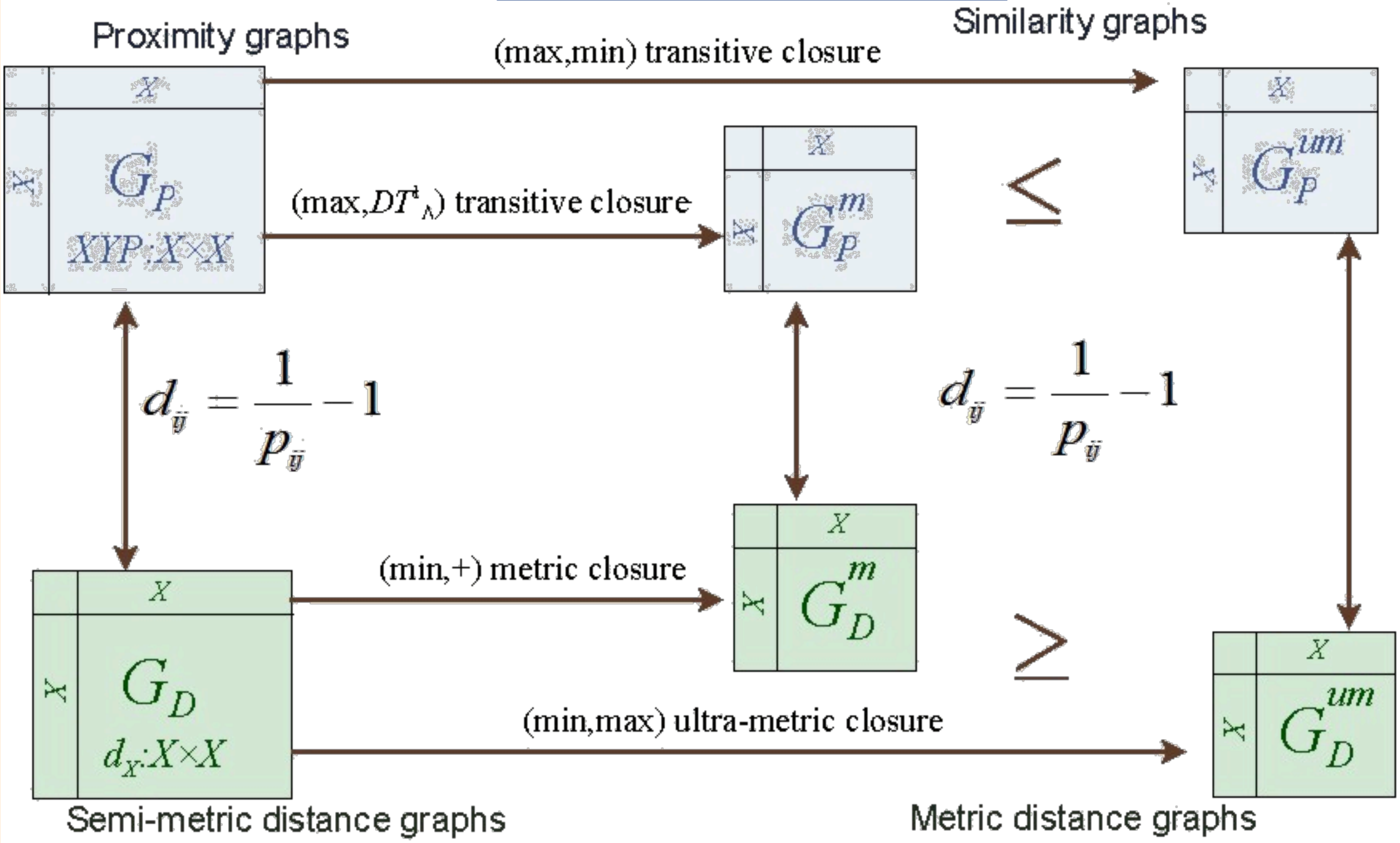
most agressive

shortest-path where ***path length*** is weakest link



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Simas & Rocha [2014]. *Network Science*. In Press. arXiv:1312.2459

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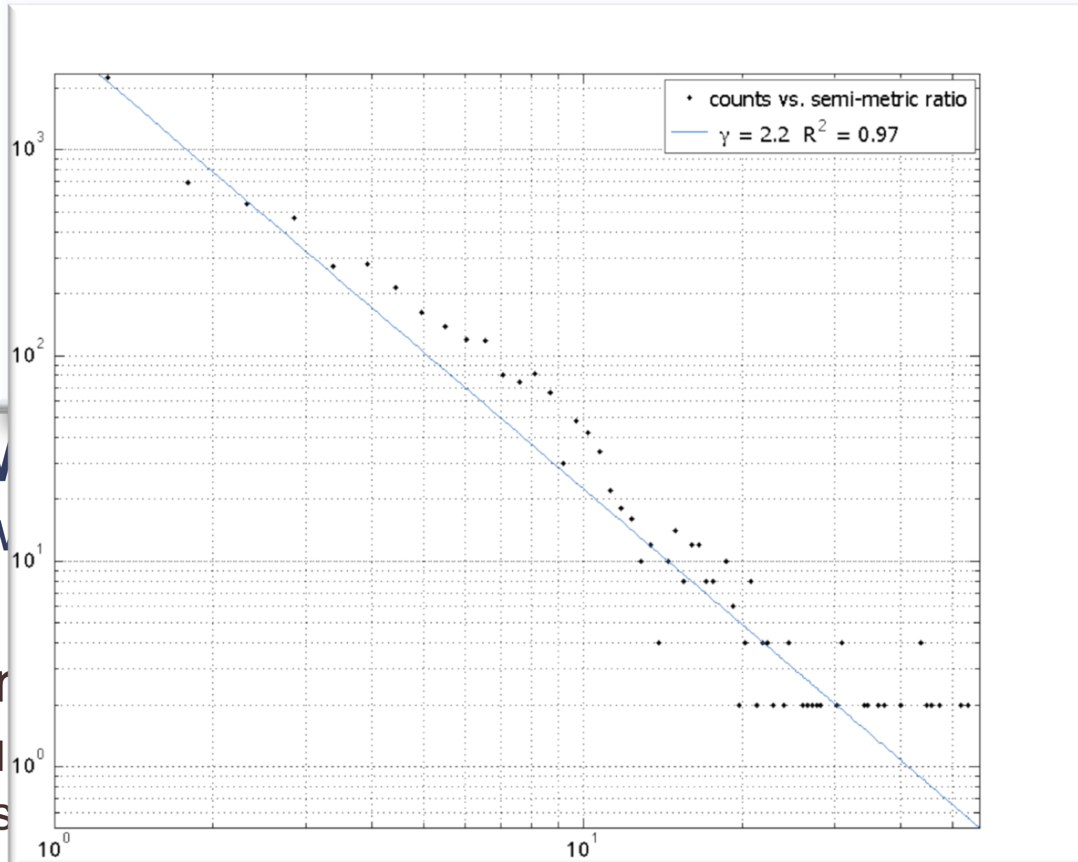
- **Semi-metric (semi-triangular) edges**:
  - Redundant for shortest-path computation (distance closure)
  - Null edge betweeness centrality
  - Varying *semi-metric distortion*

rity

$s\downarrow i,j = d\downarrow i,j$,



M b-graph for

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subgraph, transitive reduction)

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d^{mc}

d_b

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Simas, Ciampaglia, Sporns & Rocha [2014]. In Preparation.

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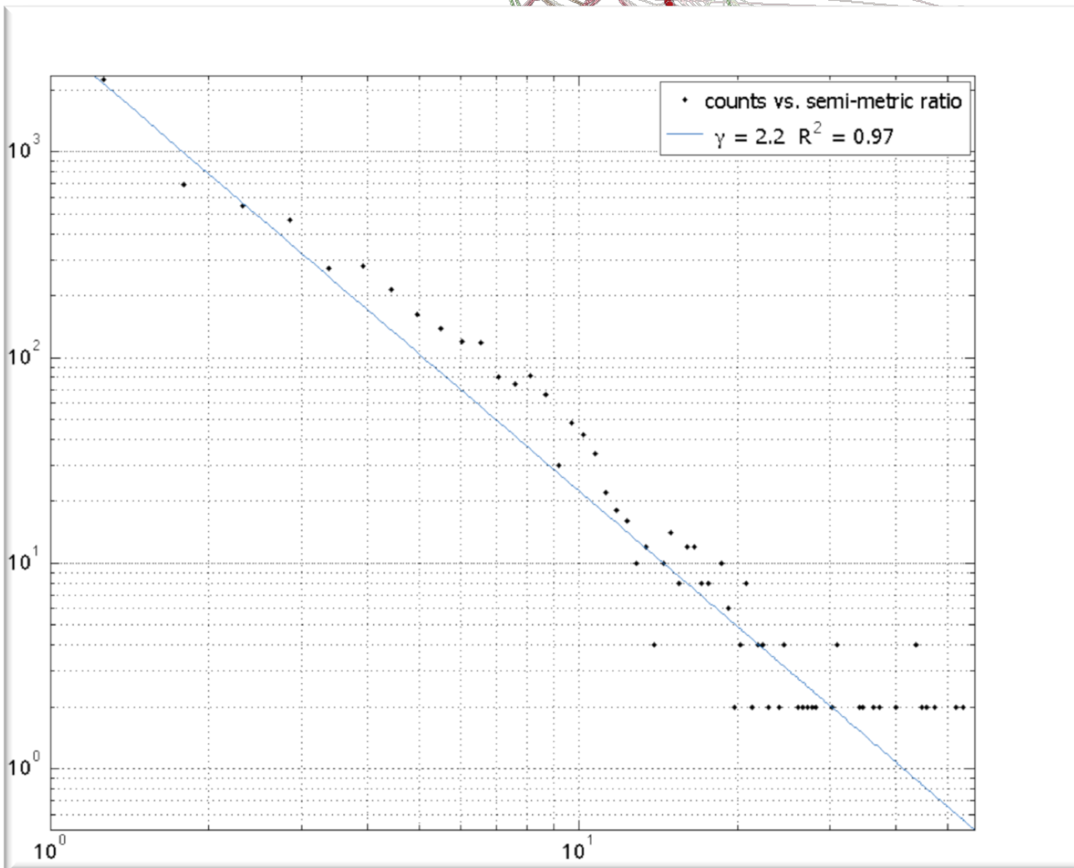
US airport Network

Colizza,, Pastor-Satorras,, Vespignani [2007]. *Nature Physics* **3**, 276-282.;



Available airplane seats between US cities

5% (83%) of edges
e semi-metric
(semi-ultra-metric)
and removed from backbone

Simas, T. [2012]. *PhD Thesis*. Indiana University.

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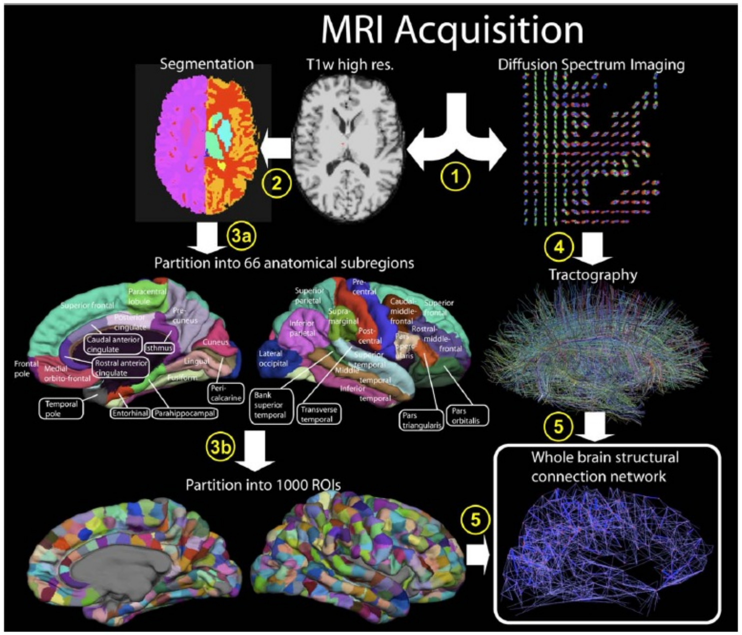
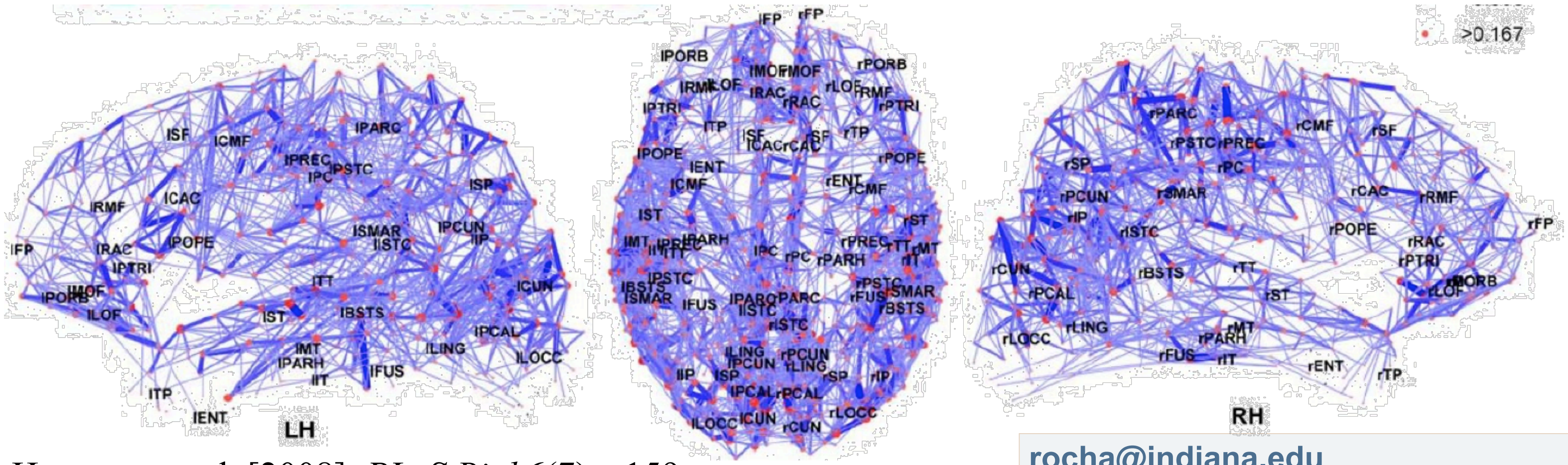
Full network



cortico-cortical axonal pathways from diffusion spectrum Imaging (DSI)

Nodes: functionally specialized regions



Hagmann et al. [2008]. *PLoS Biol* **6**(7): e159.

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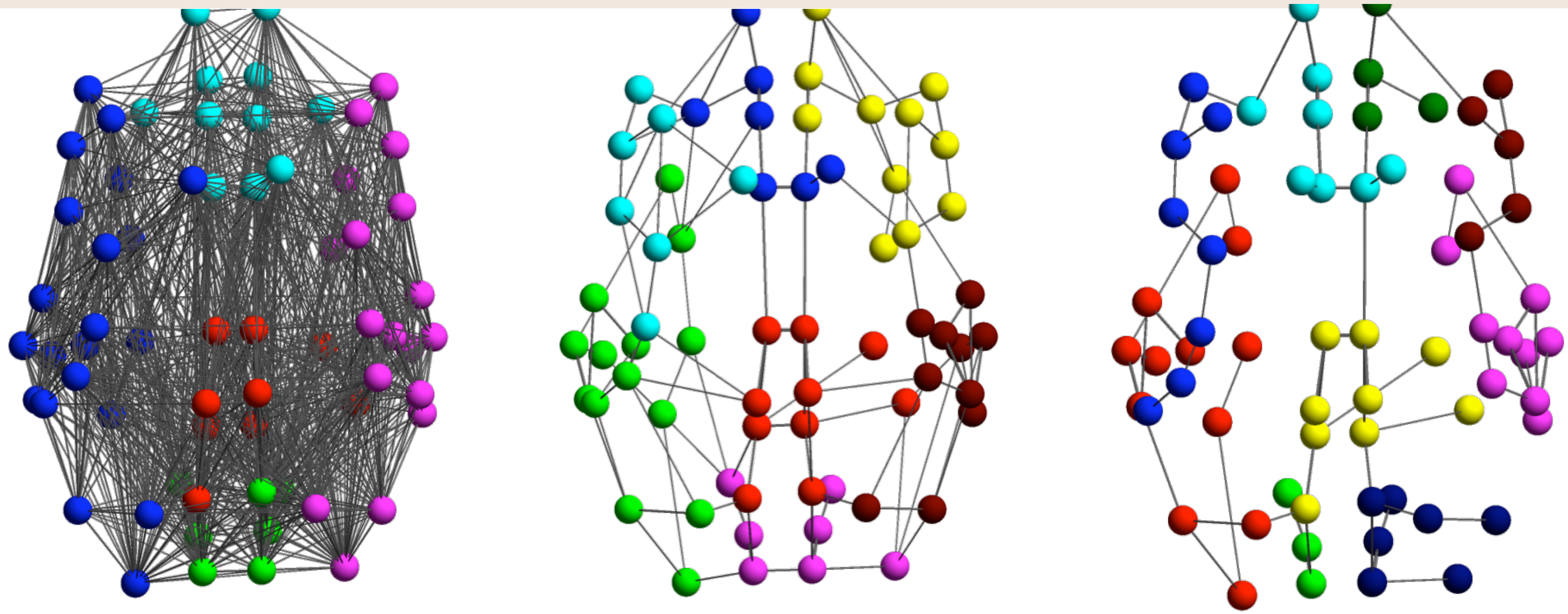
Human Cerebral Cortex Network



Original **Metric Backbone** **Ultra-Metric Backbone**

cortico-cortical axonal pathways from diffusion spectrum Imaging (DSI)

91% of edges are semi-metric (removed from backbone)!!!

94% of edges are semi-ultra-metric

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Semi-metricity and modularity

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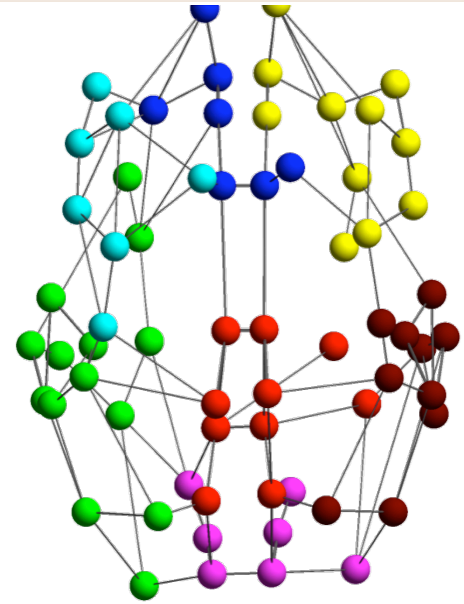
#id	Network	# Nodes	SM	USM
1	USN	500	75%	83%
2	HCN	66	91%	94%
3	HBFN	116	85%	98%
4	C-Elegans	297	31%	45%
5	BKF	58	85%	91%
6	ARP-IPP	1,702	71%	88%
7	ARP-PIP	382	73%	93%
8	ARP-Keywords	500	96%	99%
9	WordNet	150	85%	93%
10	SCN	12,722	9%	28%
11	APN	14,845	20%	48%
12	HEN	5,835	13%	34%



Metric Backbone

Ta
net
co
net
net

	USN	HCN	HBFN	C-Elegans	BKF	ARP-IPP	ARP-PIP	ARP-Keywords	WordNet	SCN	APN	HEN
NET	0.6175	0.7165	1	0.1691	0.7474	0.7374	0.6265	0.9925	0.4247	0.6517	0.6696	0.5062
MB	0.2335	0.1318	0.4783	0.1261	0.2482	0.2832	0.2866	0.1950	0.1269	0.6165	0.6077	0.4600
UMB	0.2335	0.0.0	0.0	0.1115	0.1412	0.1359	0.0913	0.0093	0.0214	0.6165	0.6077	0.4600

work; APN - LANL co-citation
citation scientific collaboration

Simas, Ciampaglia, Sporns & Rocha [2014]. In Preparation.

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automatic fact checking: can machines determine truth?

from data in Wikipedia

Giovanni Luca Ciampaglia

DBpedia

4.0 million “things” with 470 million “facts”.

Using *metric closure*, predicts democrat from republican politician with very high accuracy (also decent for geography, capitals director, academy awards)

Johan Bollen

Fil Menczer

Alessandro Flammini

Massive graph (V = 3.14M; E = 23M) is extremely semimetric (98%)

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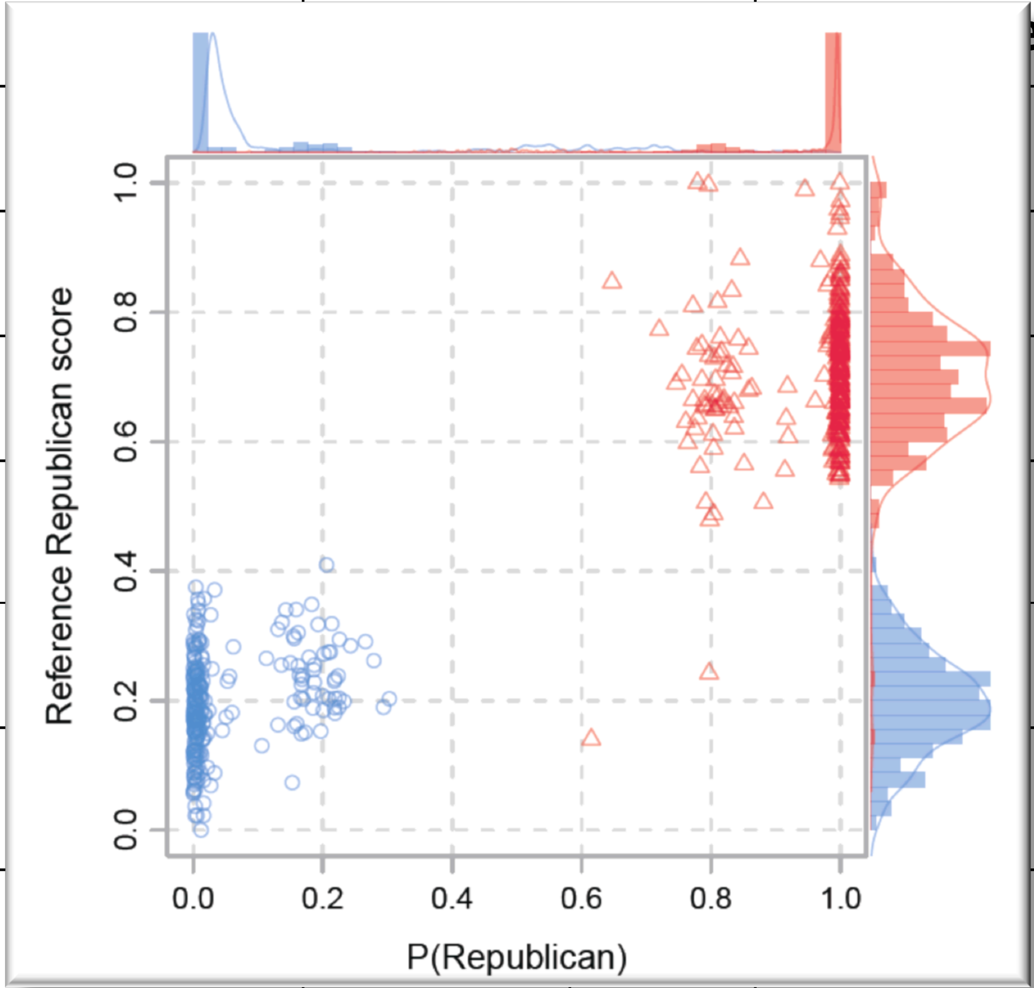
AUC

				ected	
					RF
House					54%
					99%
					57%
Senate					55%
					100%
					61%



Baseline: original graph with no closure

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complex adaptive systems

CASCI Team

and computational intelligence @ indiana university,
http://casci.informatics.indiana.edu

luis m. rocha (PI)

- computation as a general principle for generating open-ended complexity (in embodied systems)
  - Turing/Von Neumann principle of universal computation/ self-replication is most fundamental principle of life: evolution via genetic variation and selection.
- general questions deriving from this evolutionary principle
  - How do cells and collectives of cells compute?
  - How can artificial systems evolve?
  - How does external language extend cognition?
  - Can we understand and control collective intelligence via external language? Does it evolve?
- projects focus on language and information on networks
  - dynamics in complex networks, automata dynamics, network topology, text mining for translational biomedicine, computational biology, agent-based modeling, artificial life, evolutionary systems, collective intelligence

and computational biology
@ instituto gulbenkian de ciência, portugal

“Let the whole outside world consist of a long paper tape”. —John von Neumann, 1948

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selected projects – text, literature, and social media mining

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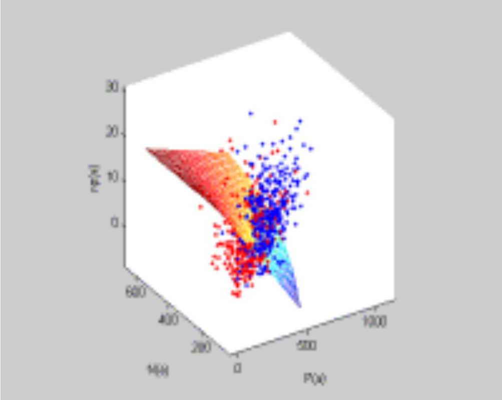
Content Extraction and Event Detection: Protein-Protein Interaction, Drug-Drug-interaction, Drug Pharmacokinetics, Numerical Parameter, Event Prediction from Twitter data, Protein Structure Prediction, etc. Among top performing teams in BioCreative PPI tasks

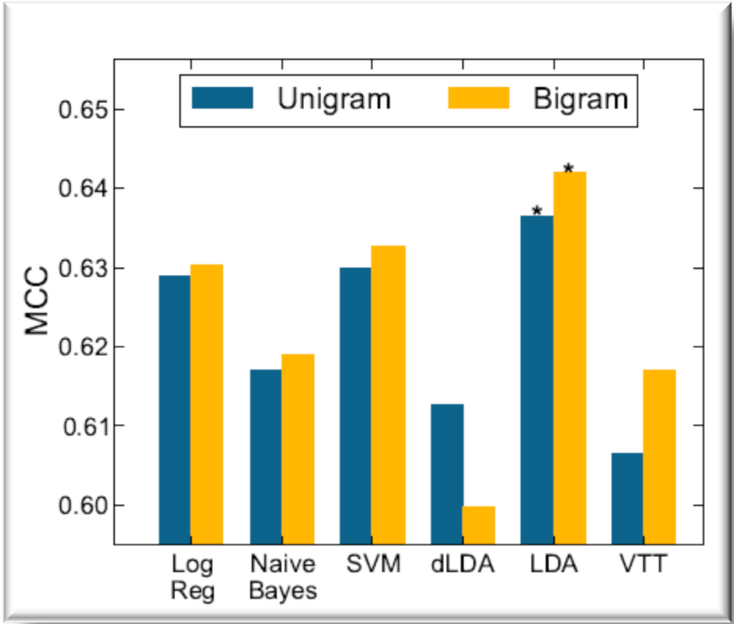


Wu et al [2013]. *BMC Bioinformatics*, **14:**35.

Wang, et al [2009]. *J. Biomedical Informatics*. **42** (4): 726-735.

Abi Haidar, A et al. [2008] *Genome Biology* **9**(Suppl 2):S11.

Verspoor, K., et al [2005]. *BMC Bioinformatics*, 6(Suppl 1):S20.



Text Classification: Retrieval of relevant documents, tweets, profiles, etc.

Lourenco, et al [2011]. *BMC Bioinformatics.* **2**(Suppl 8):S12

Abi-Haidar & L.M. Rocha [2011]. *Evol. Intel.* **4**(2):69-80.

Kolchinsky, et al [2010]. *Trans. Comp. Bio. Bioinf.*, **7**(3):400-411

Kolchinsky et al [2013]. PSB **18**:409-420.

Kolchinsky et al [2014]. *PLoS One*. In Press.

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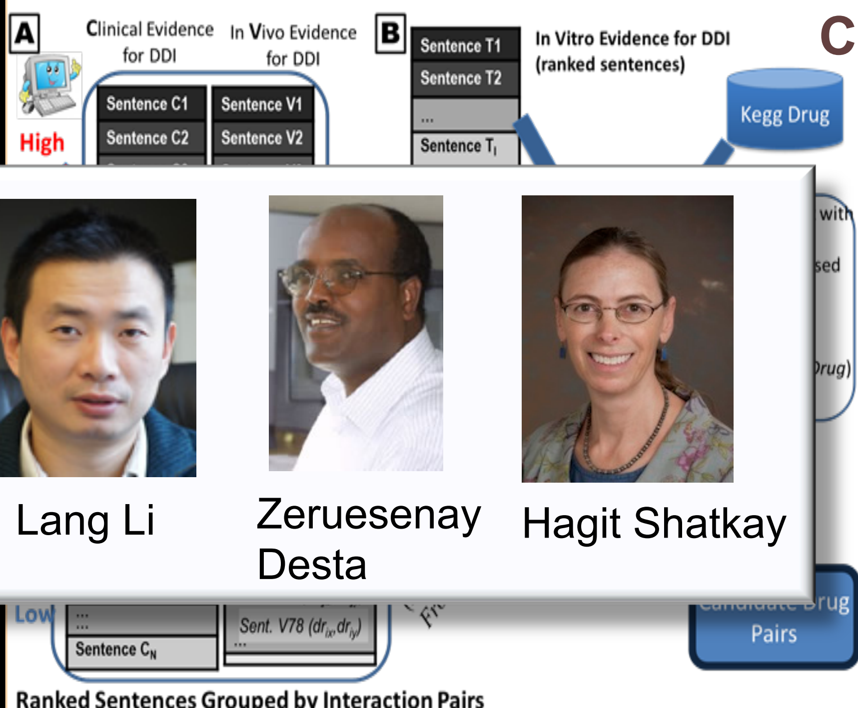
classification and extraction of evidence from the Bibliome

threat to public health: drug-drug interaction (DDI) is major cause of *adverse drug reaction* (ADR). ≈ 195K/year hospitalizations and 74K/year emergency room visits in US. Expected to increase with *polypharmacy*.

DDI experimental evidence: *in vitro*, molecular interactions within cell; *in vivo*, whether molecular interaction impacts drug exposure in humans; *clinical*, whether DDI changes human response to drugs (efficacy, ADR).

Knowledge gaps: missing evidence of any of the three types. **Need to link evidence** of molecular to clinical DDI, at collective intelligence level



Lang Li

Zeruesenay Desta

Hagit Shatkay

Corpora development and Text Classification of evidence: abstracts and sentences with evidence of DDI of one type to fill ***knowledge gaps***

Kolchinsky et al [2013]. PSB **18**:409-420.

Wu et al [2013]. *BMC Bioinformatics*, **14**:35. DOI:10.1186/1471-2105-14-35.

Kolchinsky et al [2014]. *PLOS One*. In Press.

Wu et al [2014]. *J. Biomed. Informatics,* Submitted.

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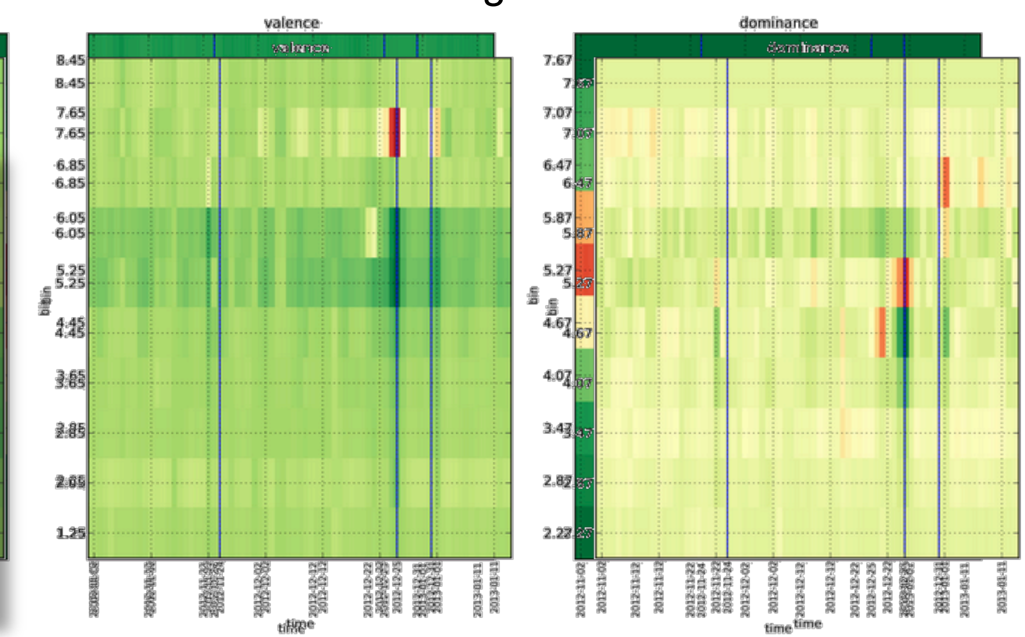
studying collective behavior

eigenmoods from text records on social media

- text as external component of collective behavior
  - patterns of text used by collectives
    - rather than individual brains and genes
  - e.g. Collective mood behavior on Twitter
    - Sex search data
    - Situations with divergent collective moods

ANEW Twitter measurements 2012

Reconstructed matrix after first singular vector removed



Johan Bollen

Joana Sá

Wood et al [2014]. *In Preparation.*

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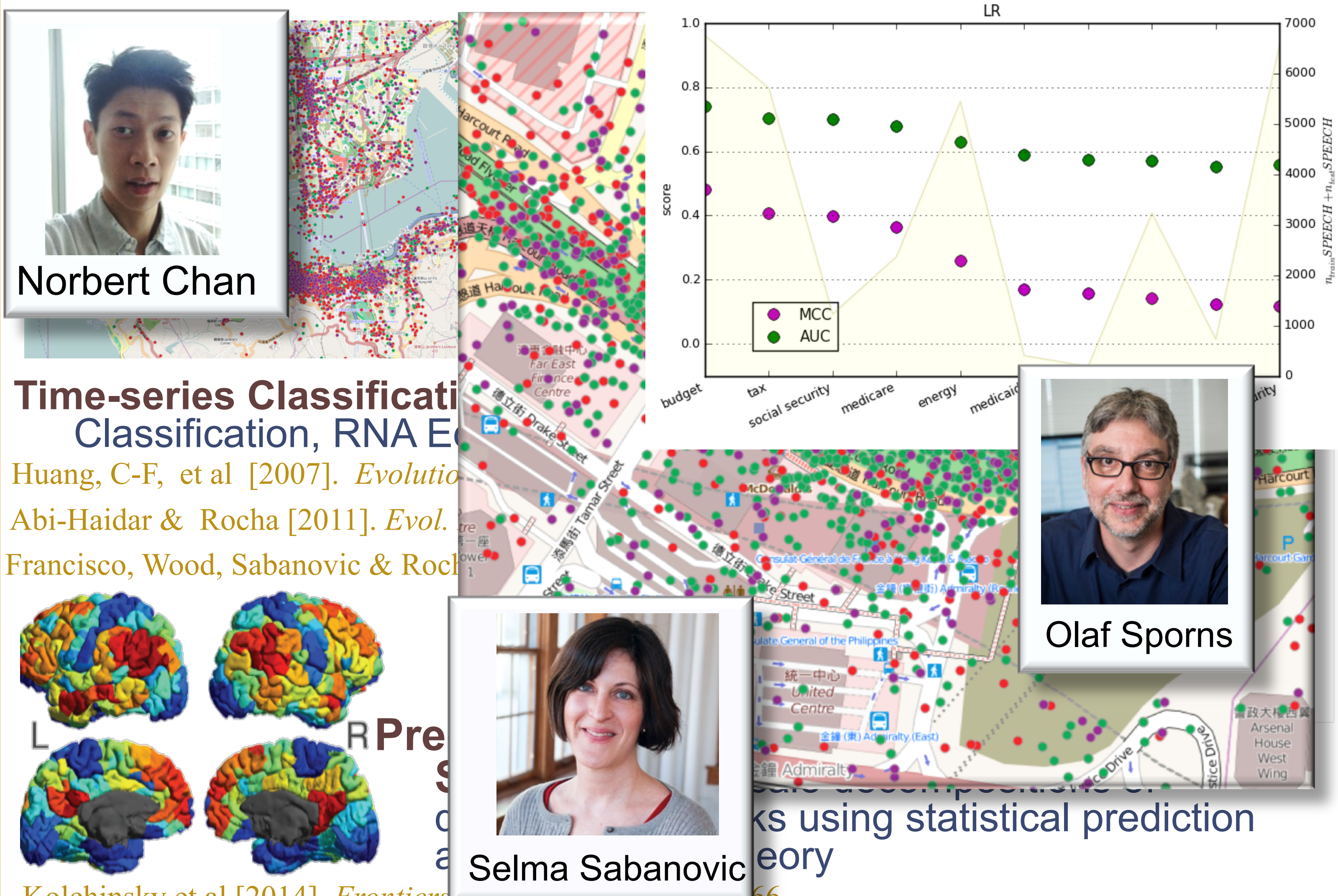
Selected projects

Political activity: social unrest via Instagram and polarization in congress



Time-series Classificati
Classification, RNA E

Huang, C-F, et al [2007]. *Evolutio*

Abi-Haidar & Rocha [2011]. *Evol.*

Francisco, Wood, Sabanovic & Roc

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ks using statistical prediction
eory

Kolchinsky et al [2014]. *Frontiers* ... :66.

Kolchisnky & Rocha [2011]. *ECAL 2011*: 423-430.

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Boolean networks, sound, art, and education

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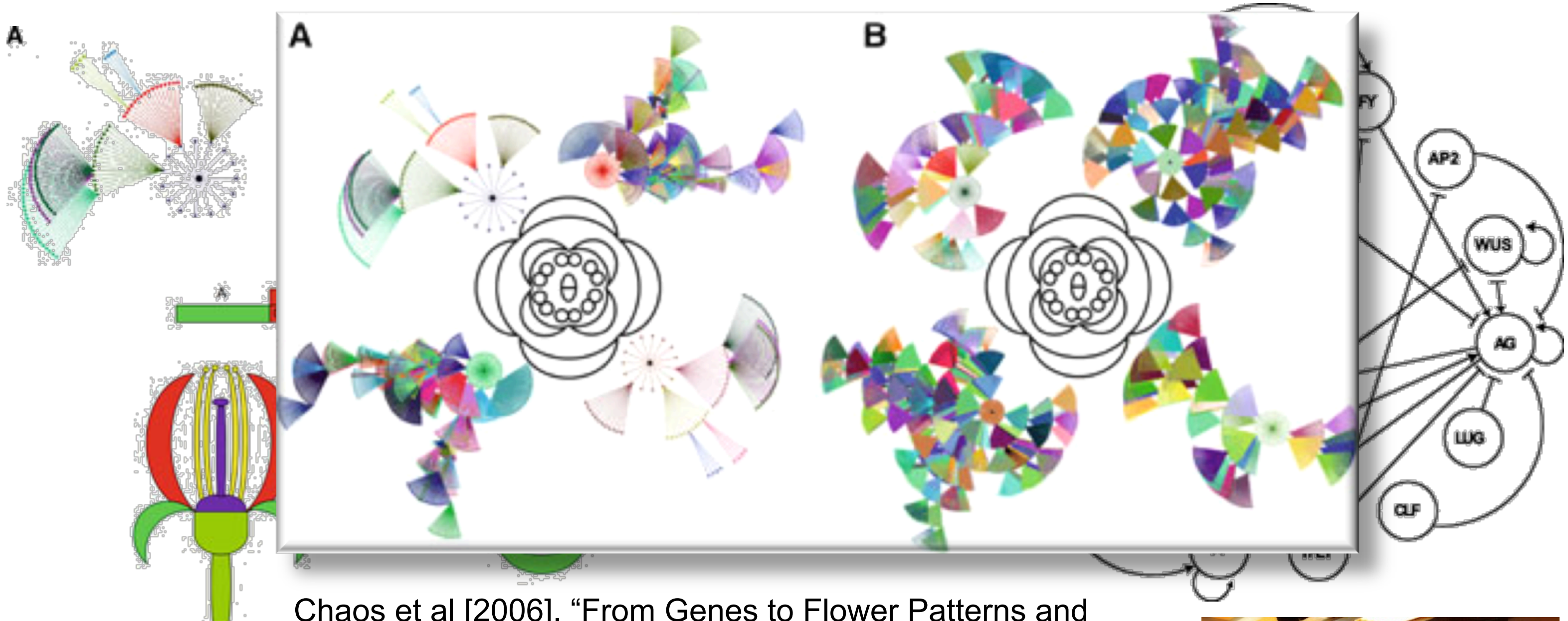
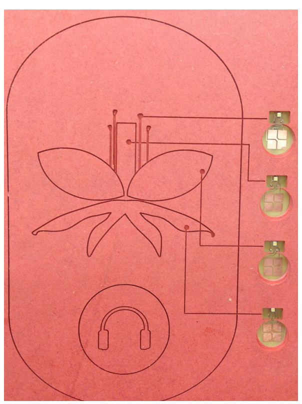
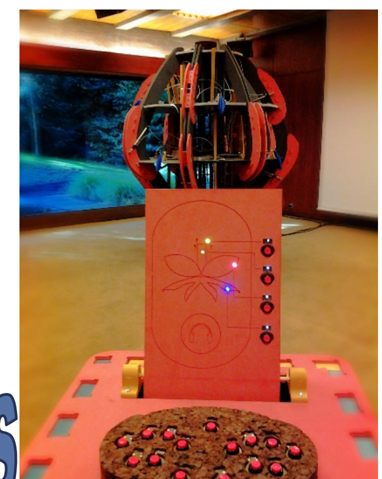


Chaos et al [2006]. "From Genes to Flower Patterns and Evolution: Dynamic Models of Gene Regulatory Networks". *Journal of Plant Growth Regulation*. **25**(4): 278-289





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metric closure – APSP (Dijkstra)

Proximity

X | X | G_P | $XYP: X \times X$

Rocha, Luis M. [2002]. In: *Soft Computing Agents*. V. Loia (Ed.):137-163.

Rocha, L.M. et al [2005]. *IEEE Web Intelligence* (WI'05): 565-571.

shortest-path where ***path length*** is sum of edges

φ

$$d_X(x_i, x_j) = \frac{1}{XYP(x_i, x_j)} - 1$$

X | X | G_D | $d_X: X \times X$

Distance

Metric Closure (min/+)

= metric
> semi-metric

X | X | G_D^m

(Shortest Path)

$b{\downarrow}i,j = d{\downarrow}i,j$

$s{\downarrow}i,j = d{\downarrow}i,j$

Measures of semi-metric behavior

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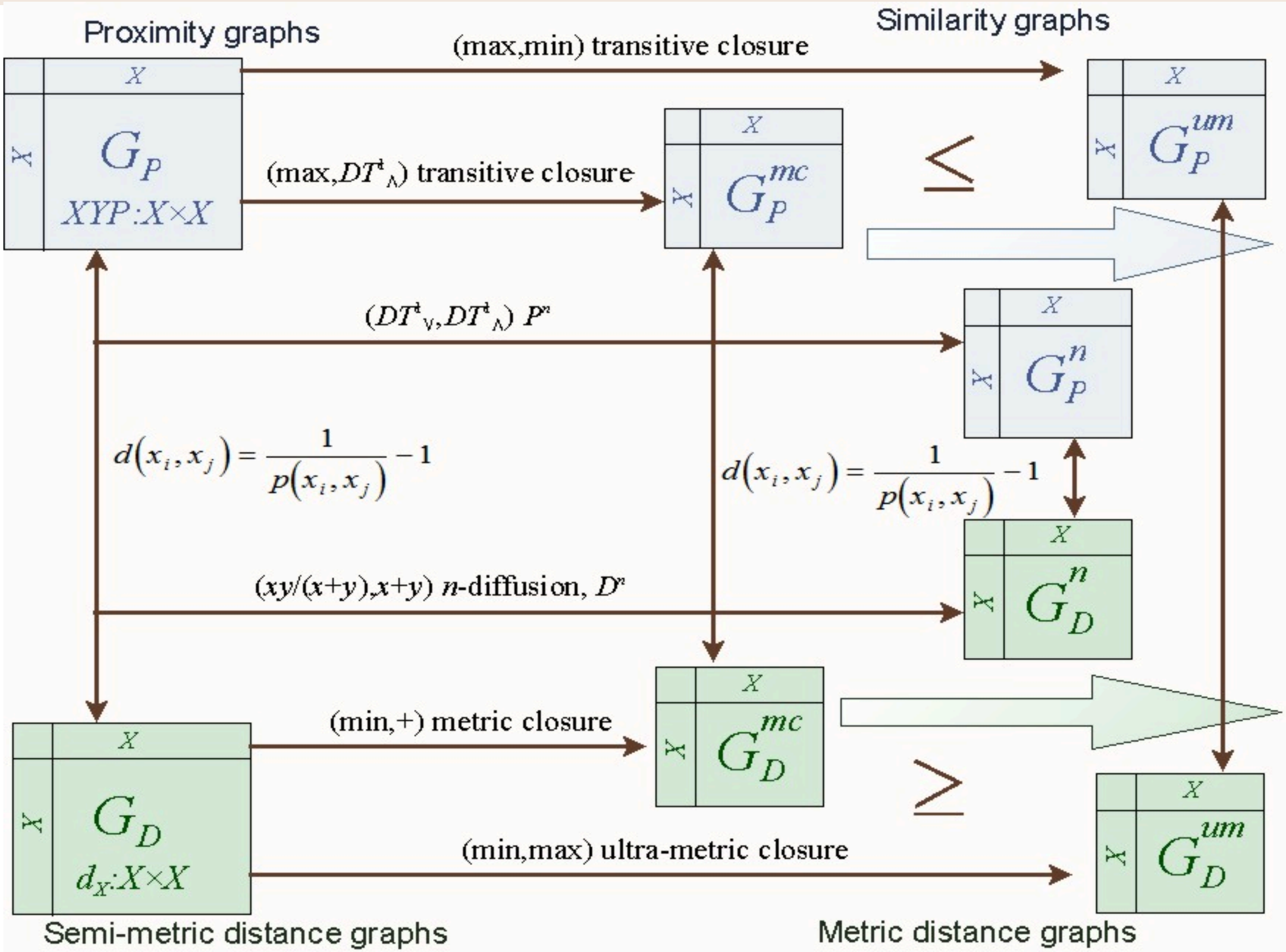
all cases



Simas & Rocha [2014]. *Network Science*. In Press. arXiv:1312.2459

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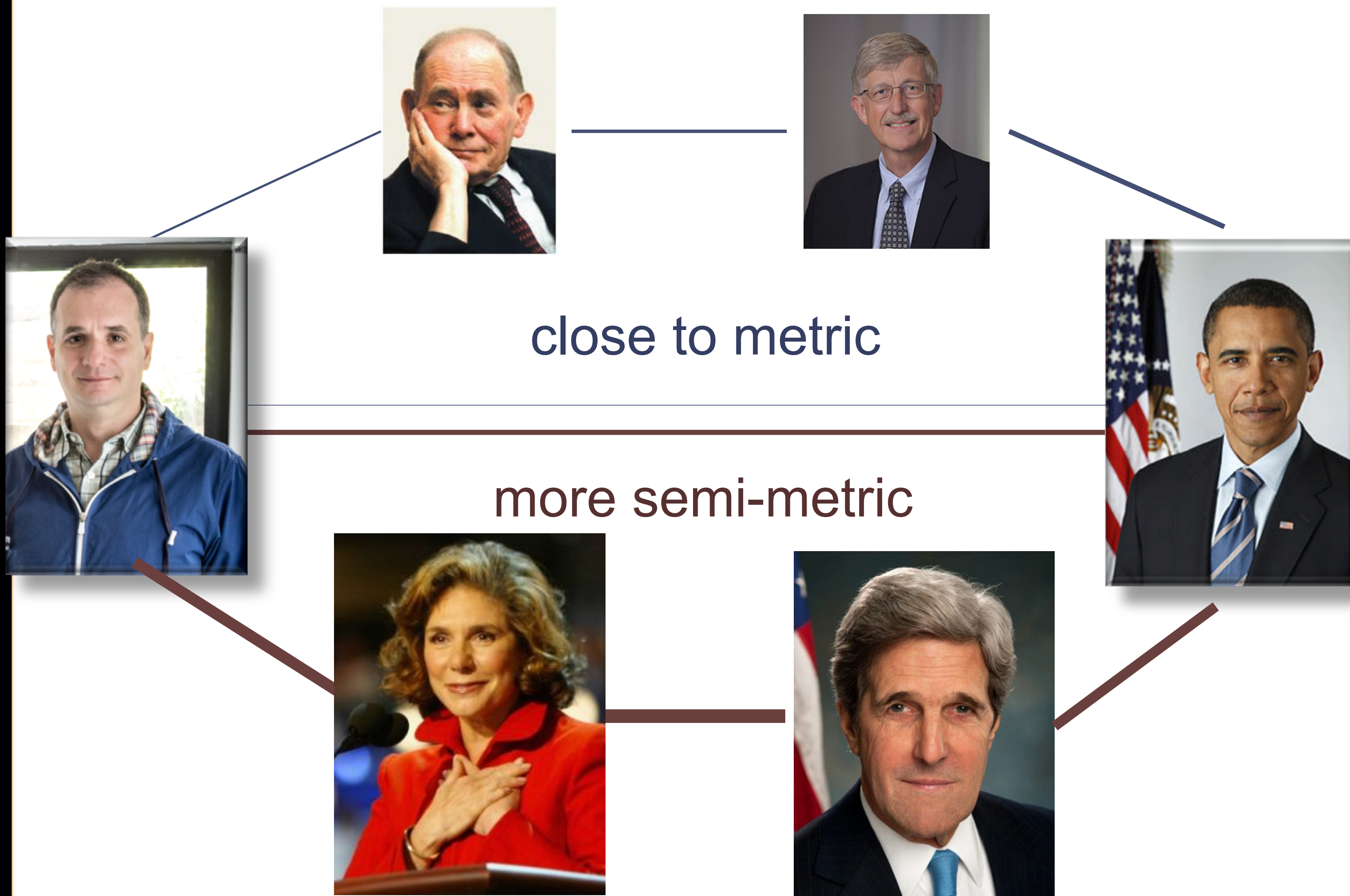
intuition about latent associations



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ultra-metric closure

intuition

- Tends to link items very strongly
- Greater distortion of original graph
- Worse for inference

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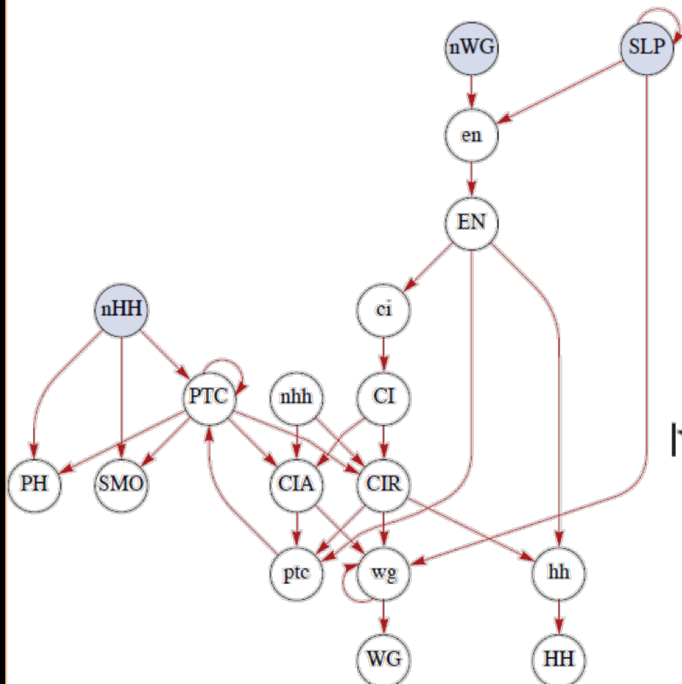
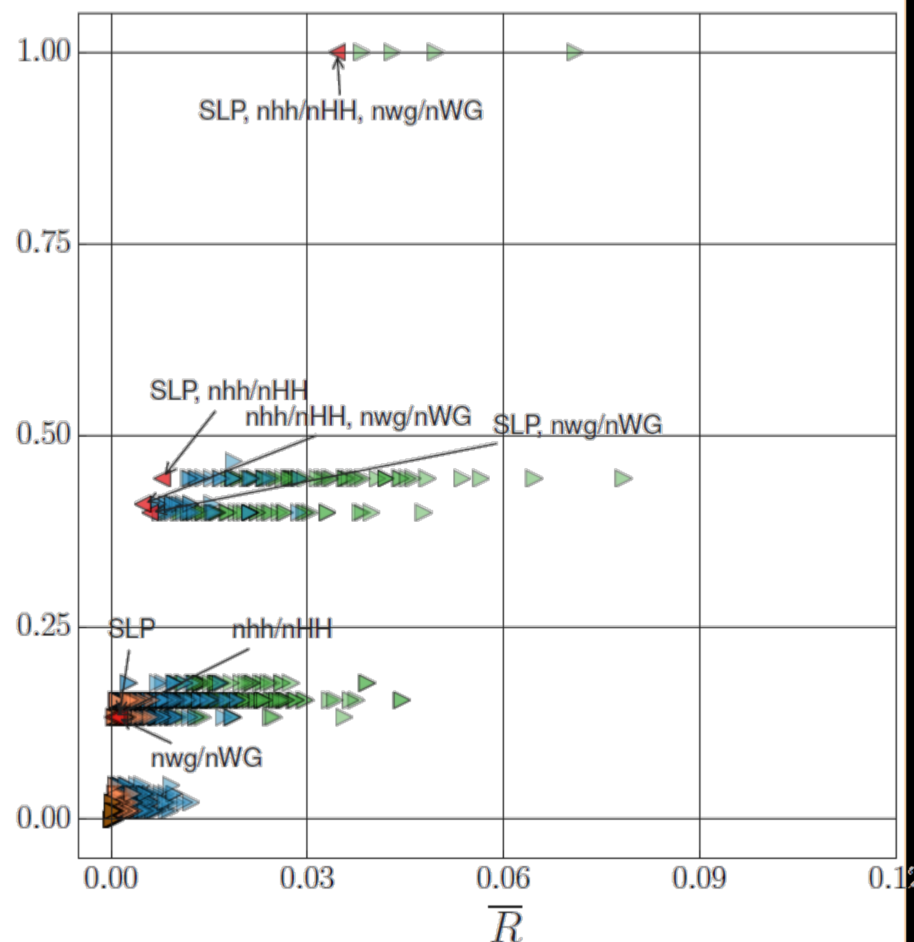
Can structural controlability uncover control?

Drosophila model (Albert et al)





4 nodes predicted by structural control:

$\{SLP, nWG, nhh/nHH, PH\}$,
$\{SLP, nWG, nhh/nHH, SMO\}$,
$\{SLP, nWG, nhh/nHH, CIR\}$,
$\{SLP, nWG, nhh/nHH, CIA\}$

Gates & Rocha [2014]. *ALIFE 2014*: 429-430.
Gates & Rocha [2014]. *In preparation..*

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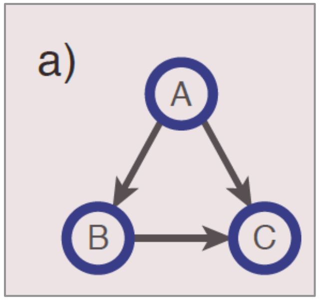
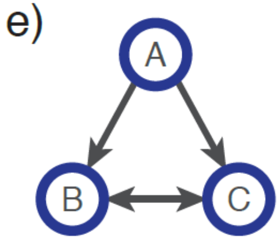
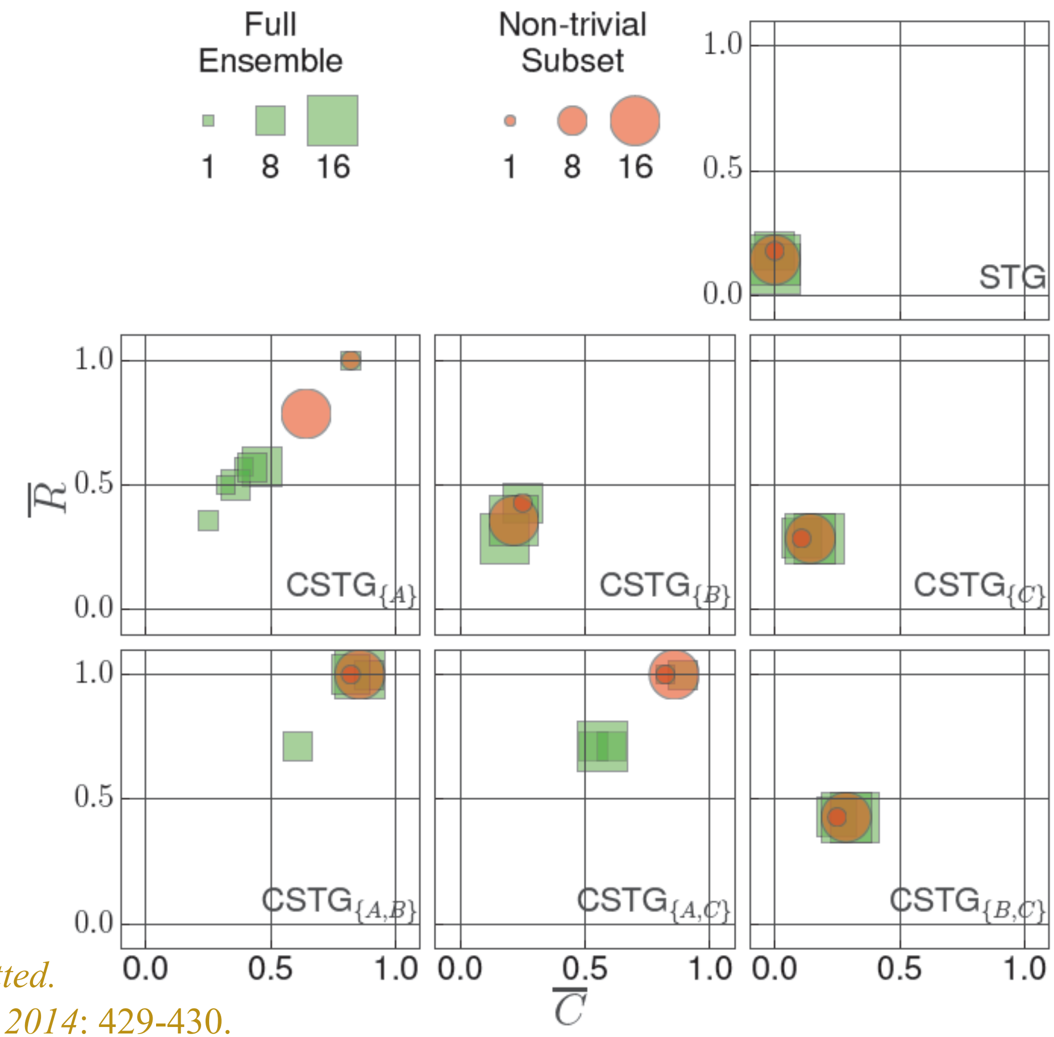
Can structural controlability uncover control?

In presence of dynamics

Consider small network motifs:







The larger the ***canalization***, the less predictable is structural control

Gates & Rocha [2014]. *Submitted.*
Gates & Rocha [2014]. *ALIFE 2014*: 429-430.