introduction to *network analysis* (*ina*)

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announcements *7th week*

- *homework #2* out *today*
- *homework #2* due in *two weeks*
- *homework #1* results *weekend*

- *project consultations online*
- *÷-vector centrality review*

- *video lectures & labs this week*
- *feedback box* from *last week*

node *mixing*

introduction to *network analysis* (*ina*)

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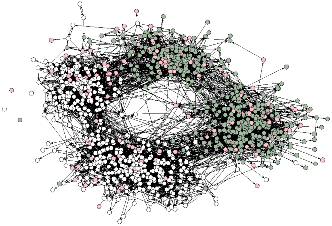
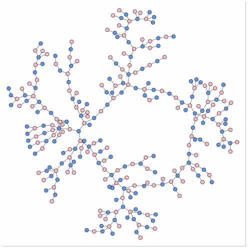
mixing *definition*

- *node mixing* are *correlations of linked* nodes
- in *assortative mixing* nodes *linked to similar* others
- in *disassortative mixing* nodes *linked to dissimilar* others



assortative mixing by age/race



(dis)assortative mixing by gender

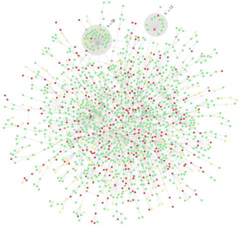
mixing *degree*

- special case of *node mixing by degree* [New02]
- majority of *social networks* is *degree assortative*
- most *other networks* are *degree disassortative*

$$p_{kk'} = k\frac{k'}{2m-1} = m\frac{kk'}{\binom{2m}{2}} \approx \frac{kk'}{2m}$$

celebrity hubs date hubs

but $10^3/10^8 = 0.00001$



protein hubs avoid hubs

but $p_{56,13} = 0.16 \gg p_{1,2} = 0.0004$

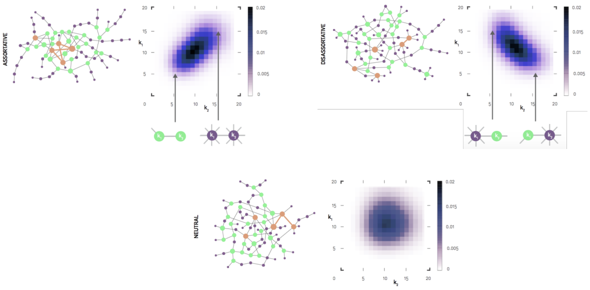
mixing *matrix*

— *endpoints degree distribution* $e_{kk'}$ defined as

- $e_{kk'}$ is *link probability* between *degree-k & -k'* nodes
- q_k is *neighbor non-excess degree distribution*

$$\sum_{kk'} e_{kk'} = 1 \qquad \sum_{k'} e_{kk'} = q_k = n_k \frac{k}{2m-1} \approx \frac{kp_k}{\langle k \rangle}$$

$e_{kk'} = q_k q_{k'}$ in *neutral networks* but impractical for (*dis*)*assortative networks*



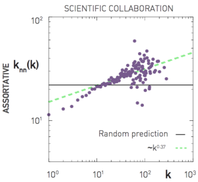
mixing *exponent*

— *neighbor degree function* k_{nn} [PSVV01] defined as

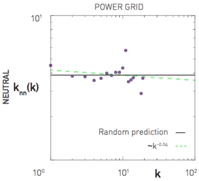
- k_{nn} is *average neighbor degree* of *degree-k* nodes
- $\mathrm{P}(k'|k)$ is *link probability* of *degree-k to -k'* node
- μ is *degree mixing power-law exponent* [VPSV02]

$$k_{nn}(k) = \sum_{k'} k' \mathrm{P}(k'|k) = \sum_{k'} k' \frac{e_{kk'}}{\sum_{k'} e_{kk'}}$$

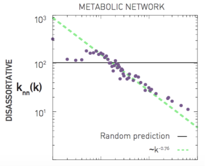
$k_{nn} = \frac{\langle k^2 \rangle}{\langle k \rangle}$ in *neutral networks* and $k_{nn}(k) \sim k^{\mu}$ in *(dis)assortative networks*



$\mu = 0.37 \pm 0.11$



$\mu = 0.04 \pm 0.05$



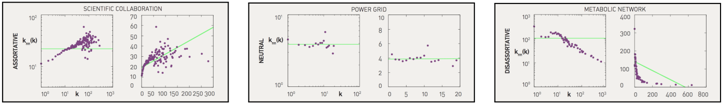
$\mu = -0.76 \pm 0.04$

mixing *coefficient*

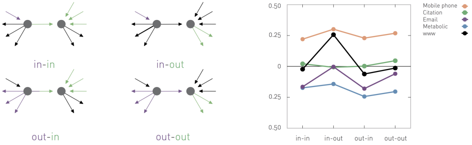
- *degree mixing coefficient* r [New02, Est11] defined as
  - r is *correlation* of *linked nodes' degrees* [New03]
  - q_k is *neighbor excess degree distribution*

$$r = \sum_{kk'} \frac{kk'(e_{kk'} - q_k q_{k'})}{\sum_k k^2 q_k - \left(\sum_k k q_k\right)^2}$$

$r = 0$ in *neutral networks* and $k_{nn}(k) \sim rk$ in (*dis*)*assortative networks*



$r = 0.13$ $\quad$ $r = 0$ $\quad$ $r = -0.04$

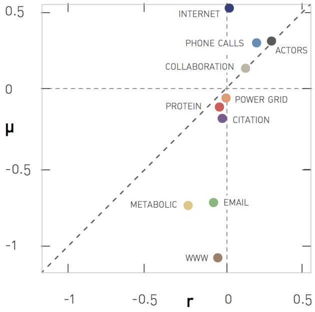


mixing *networks*

— *coefficient & exponent* r & μ in real networks [Bar16]

— r & μ *correlate* in *assortative* regime and $\mathrm{sgn}(r) = \mathrm{sgn}(\mu)$

NETWORK	N	r	μ
Internet	192,244	0.02	0.56
WWW	325,729	-0.05	-1.11
Power Grid	4,941	0.003	0.0
Mobile Phone Calls	36,595	0.21	0.33
Email	57,194	-0.08	-0.74
Science Collaboration	23,133	0.13	0.16
Actor Network	702,388	0.31	0.34
Citation Network	449,673	-0.02	-0.18
E. Coli Metabolism	1,039	-0.25	-0.76
Protein Interactions	2,018	0.04	-0.1



mixing *structural*

— *structural disassortativity* $\frac{E_{kk'}}{m_{kk'}} > 1$ [MSZ04] in real networks

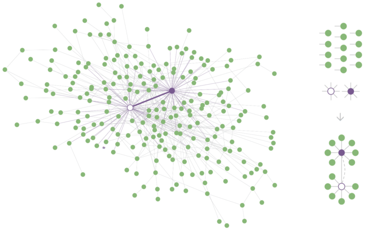
– $E_{kk'}$ is *number of links* between *degree-k & -k'* nodes

– $m_{kk'}$ is *maximum* $E_{kk'}$ hence $\min(kn_k, k'n_{k'}, n_k n_{k'})$

$$E_{kk'} = 2me_{kk'} = \langle k \rangle n e_{kk'}$$

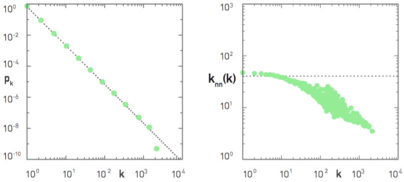
natural cutoff $k_{max} \sim n^{\frac{1}{\gamma-1}}$ and *structural cutoff* $k_s \sim \sqrt{\langle k \rangle n}$

— *structural disassortativity* in *scale-free* networks with $\gamma < 3$

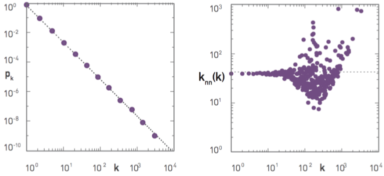


$k = 55$ and $k' = 46$ then $E_{kk'} = 2.81 > 1$

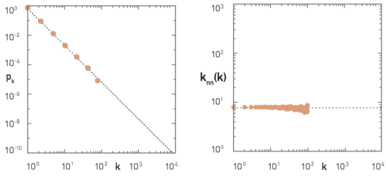
mixing *scale-free*



configuration *scale-free* network as *simple graph*

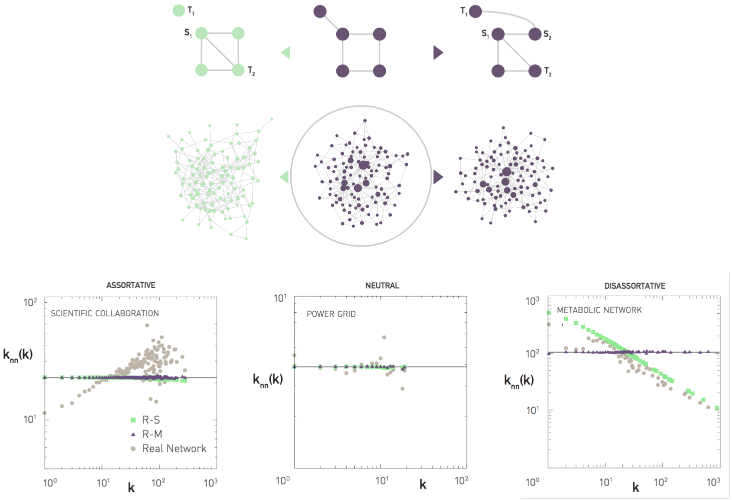


configuration *scale-free* network as *multigraph*



configuration *scale-free* network *without* ***hubs*** $k \geq k_s$

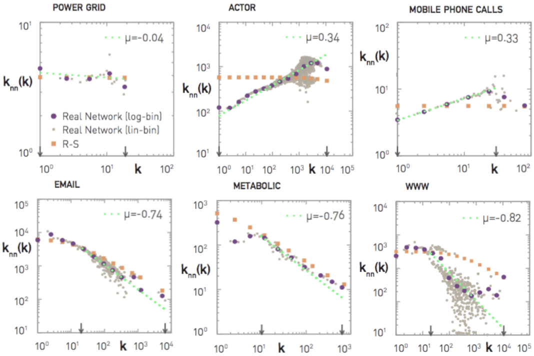
mixing *randomization*



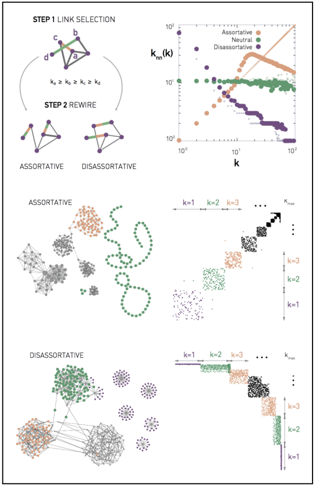
degree-preserving randomization with *simple/multi links* retains/destroys *structural disassortativity*

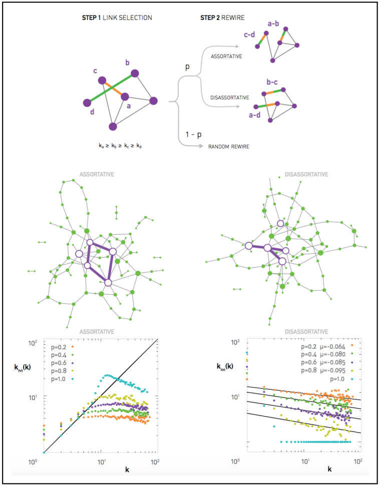
mixing *networks*

- *neighbor degree* k_{nn} in real networks [Bar16]
- *collaboration assortative* and *technological neutral*
- *biological/information (structurally) disassortative*



mixing *models*

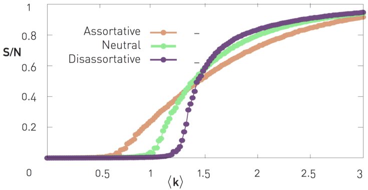


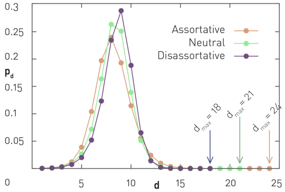


(dis)assortative degree-preserving randomization [XBS05]

mixing *impact*

- *degree mixing* impacts *connectivity* and *distances* [New02]
- *assortative mixing* coexists with *community structure* [NP03]
- *mixing* influences *resilience* [VM03] and *controllability* [LSB11]





mixing *references*

A.-L. Barabási.
Network Science.
Cambridge University Press, Cambridge, 2016.

Ernesto Estrada and Philip A. Knight.
A First Course in Network Theory.
Oxford University Press, 2015.

Ernesto Estrada.
Combinatorial study of degree assortativity in networks.
Phys. Rev. E, 84(4):047101, 2011.

Yang-Yu Liu, Jean-Jacques Slotine, and Albert-Laszlo Barabasi.
Controllability of complex networks.
Nature, 473(7346):167–173, 2011.

Sergei Maslov, Kim Sneppen, and Alexei Zaliznyak.
Detection of topological patterns in complex networks: Correlation profile of the internet.
Physica A, 333:529–540, 2004.

M. E. J. Newman.
Assortative mixing in networks.
Phys. Rev. Lett., 89(20):208701, 2002.

M. E. J. Newman.
Mixing patterns in networks.
Phys. Rev. E, 67(2):026126, 2003.

Mark E. J. Newman.
Networks: An Introduction.
Oxford University Press, Oxford, 2010.

mixing *references*

M. E. J. Newman and Juyong Park.
Why social networks are different from other types of networks.
Phys. Rev. E, 68(3):036122, 2003.

Romualdo Pastor-Satorras, Alexei Vázquez, and Alessandro Vespignani.
Dynamical and correlation properties of the Internet.
Phys. Rev. Lett., 87(25):258701, 2001.

Alexei Vázquez and Yamir Moreno.
Resilience to damage of graphs with degree correlations.
Phys. Rev. E, 67(1):015101, 2003.

Alexei Vázquez, Romualdo Pastor-Satorras, and Alessandro Vespignani.
Large-scale topological and dynamical properties of the Internet.
Phys. Rev. E, 65(6):066130, 2002.

R. Xulvi-Brunet and I. M. Sokolov.
Changing correlations in networks: Assortativity and dissortativity.
Acta Phys. Pol. B, 36:1431–1455, 2005.

network *fragments*

introduction to *network analysis* (*ina*)

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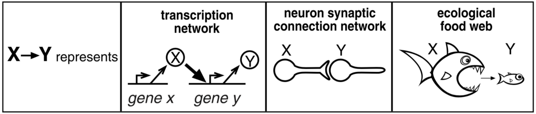
fragments *definition*

- small *subgraphs* are *building blocks* of networks
- *subgraphs* characterize *local network structure*



- *fragments* are *connected subgraphs* of networks [EK15]
- *motifs* are *frequent non-induced* fragments [MSOI$^+$02]
- *graphlets* are *arbitrary induced* fragments [PCJ04]

see mfinder and orca for implementations

network *motifs*

introduction to *network analysis* (*ina*)

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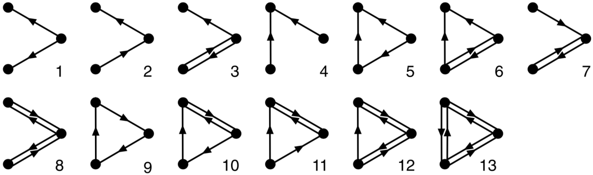
motifs *definition*

- *fragments* characterize *network-wise local structure*
- *motifs* are *frequent non-induced fragments* [MSOI+02]

  probability of *motif appearing in random graph*
  equal or greater number of times is < 0.01
- (*un*)*directed motifs* consisting of *three to five nodes*



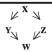
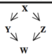
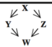
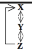
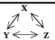
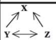
all 13 directed three-node motifs

motifs *significance*

- *motif significance* Z with *normal distribution* $N(0,1)$
  - $\widetilde{n}_i$ is *number of motifs* i in *random graph* with *variance* $\widetilde{\sigma}_i^2$
  - n_i is *number of motifs* i in *real network*

$$Z_i = \frac{n_i - \langle\widetilde{n}_i\rangle}{\widetilde{\sigma}_i} \qquad\qquad n_i - \langle\widetilde{n}_i\rangle > 0.1\langle\widetilde{n}_i\rangle$$

- $\widetilde{n}/\widetilde{\sigma}$ estimated by *motif preserving randomization* [MSOI⁺02]

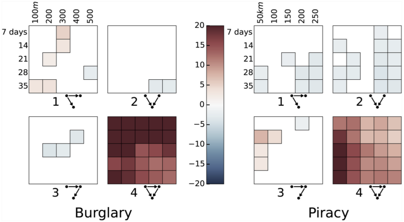
Network	Nodes	Edges	N_{real}	$N_{\text{rand}} \pm \text{SD}$	Z score	N_{real}	$N_{\text{rand}} \pm \text{SD}$	Z score	N_{real}	$N_{\text{rand}} \pm \text{SD}$	Z score
Neurons					**Feed-forward loop**			**Bi-fan**			**Bi-parallel**
C. elegans†	252	509	125	90 ± 10	3.7	127	55 ± 13	5.3	227	35 ± 10	20
Food webs					**Three chain**			**Bi-parallel**			
Little Rock	92	984	3219	3120 ± 50	2.1	7295	2220 ± 210	25			
Ythan	83	391	1182	1020 ± 20	7.2	1357	230 ± 50	23			
St. Martin	42	205	469	450 ± 10	NS	382	130 ± 20	12			
Electronic circuits (forward logic chips)					**Feed-forward loop**			**Bi-fan**			**Bi-parallel**
s15850	10,383	14,240	424	2 ± 2	285	1040	1 ± 1	1200	480	2 ± 1	335
s38584	20,717	34,204	413	10 ± 3	120	1739	6 ± 2	800	711	9 ± 2	320
s38417	23,843	33,661	612	3 ± 2	400	2404	1 ± 1	2550	531	2 ± 2	340
World Wide Web					**Feedback with two mutual dyads**			**Fully connected triad**			**Uplinked mutual dyad**
nd.edu§	325,729	1.46e6	1.1e5	2e3 ± 1e2	800	6.8e6	5e4±4e2	15,000	1.2e6	1e4 ± 2e2	5000

motifs *networks*

motif Z-scores of class *software networks* [VS05]

Network	Nodes	Edges	N_{real}	N_{rand}	Z_{score}	N_{real}	N_{rand}	Z_{score}	N_{real}	N_{rand}	Z_{score}	N_{real}	N_{rand}	Z_{score}	N_{real}	N_{rand}	Z_{score}
Software Networks (medium)					FFL S38			Bi-parallel S904			FFL extended S344						
Fairuse	106	180	41	11.6±3.3	8.94	18	7.3±3.5	3.01	33	9.5±5.5	4.25						
Aime	143	319		n/a		230	30.8±19	10.46	55	31.8±9.3	2.49						
Filezilla221a	186	331	77	29.4±6.1	7.86	30	10.2±4.5	4.38		n/a							
Aztec	255	391	68	26±5.4	7.82	25	10.6±4.6	3.15	68	14±5.9	9.08						
Exult	261	504	107	56.3±8.4	6.01	86	30.2±8	6.75	182	80.2±19.6	5.18						
Software Networks (large)					Bi-fan S204			Bi-parallel S904			Multi-X S2252			Multi-Z S206			Multi-Y S2190
blender226	495	834	486	138±30.3	11.4	33	16±5.2	3.2	123	7.8±5.8	20	22	3.7±3.6	5.04	18	4.2±3.2	4.37
gtk221	748	1147	644	189±33.8	13.4	119	25±7.5	12.5	173	26±16.7	8.8	21	2.0±1.7	10.9	19	4.2±2.7	5.41
vtk	771	1362	512	262±39.9	6.27	295	69±14.3	15.8	41	6.3±3.2	10.7	193	27.7±14.7	11.2	122	12.8±5.8	18.7
java2	1364	1947	816	189±35.5	17.7	173	48±10.8	11.5	345	18.4±14	23.3	22	2.2±2.1	9.5	17	3.8±2.2	5.99
prorally	1993	4987	22750	1840±171	122	3848	322±34.2	103.1	1080	144±50.6	18.4	210	28.7±9.2	19.8	1318	55.5±14.7	85.9
Software Networks (large)					FFL S38			S472			Multi-X incomp. S2186			Multi-X incomp S408			FFL extended S344
blender226			126	33.8±6.1	15		N/A		1976	766±162	7.43	436	196±65	3.7	94	26.2±8.6	7.88
gtk221			118	47.7±9.6	7.31	15	3.1±2.3	5.06	4177	1941±398	5.6	1462	748±261	2.73	188	68.1±13.7	8.73
vtk			229	81.6±10.6	13.9	30	13±6.7	2.53	707	388±61.6	5.17	333	217±44	2.62	718	212.1±49.1	10.3
java2			176	46.2±9	14.4	8	1.8±1.4	4.57	10212	6346±1180	3.2	2494	1397±522	2.1	257	52.5±17.6	11.6
prorally			1169	272±21	42.6	282	30.8±10.4	24.2	25099	15482±1750	5.5	5742	4163±752	2.1	2909	736±101.4	21.4

motif Z-scores of spatio-temporal *crime networks* [DM15]



motifs *profiles*

- *motif significance profile SP* [MSOI+02] defined as
  - Z_i is *significance of motif i* in *real network*

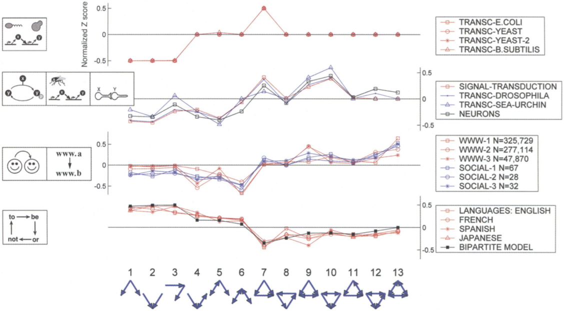
$$SP_i = \frac{Z_i}{\sqrt{\sum_i Z_i^2}} \qquad Z_i = \frac{n_i - \langle\widetilde{n}_i\rangle}{\widetilde{\sigma}_i} \qquad n_i \geq 4$$

- *motif abundance/ratio profile RP* [MIK+04] defined as
  - A_i is *abundance of motif i* in *real network*

$$RP_i = \frac{A_i}{\sqrt{\sum_i A_i^2}} \qquad A_i = \frac{n_i - \langle\widetilde{n}_i\rangle}{n_i + \langle\widetilde{n}_i\rangle + \epsilon_i} \qquad \epsilon_i = 4$$

motifs *superfamilies*

- directed *motif significance profiles* [MSOI+02]
- profiles reveal *superfamilies of real networks*



all 13 directed three-node motifs

network *graphlets*

introduction to *network analysis* (*ina*)

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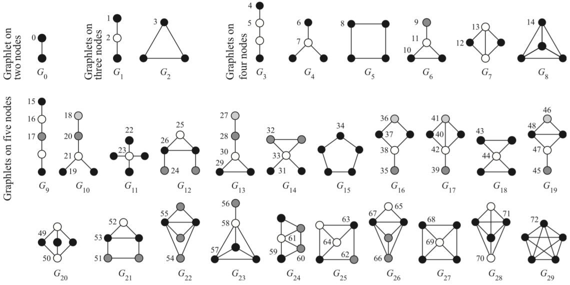
graphlets *definition*

- *fragments* characterize *node-wise local structure*
- *graphlets* are *arbitrary induced fragments* [PCJ04]
- *graphlet orbits* are *automorphisms of graphlets* [Prž07]
- (*un*)*directed graphlets* consisting of *three to five nodes*

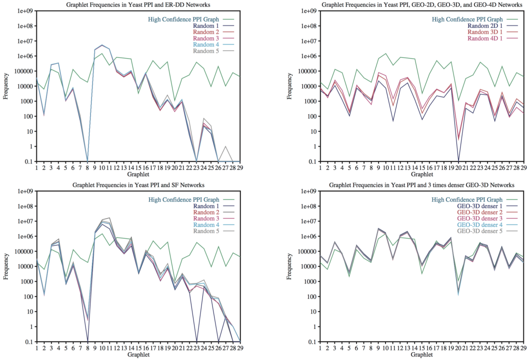


all 30 undirected two- to five-node graphlets with 73 orbits

graphlets *frequency*

- *relative graphlet frequency F* [PCJ04] defined as
  - n_i is *number of graphlets i* in *real network*

$$F_i = \frac{n_i}{\sum_i n_i}$$

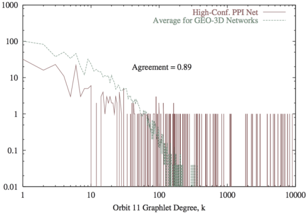


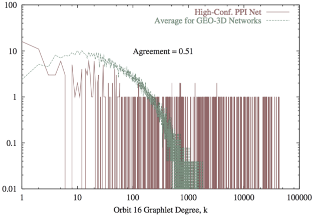
graphlet frequency in protein network and random graphs

graphlets *distribution*

- *i-th orbit graphlet degree distribution* p_k^i [Prž07] defined as
  - p_k^0 is *degree distribution* p_k of *real network*
  - p_k^i is *graphlet degree distribution* for *i-th orbit*
  - $\widetilde{p}_k^i$ is *scaled graphlet degree distribution* for *i-th orbit*

$$\widetilde{p}_k^i \sim p_k^i / k \qquad \widetilde{p}_k = \widetilde{p}_k^0 = p_k^0 = p_k$$





11th and 16th orbit graphlet degree distributions of protein network and random graph

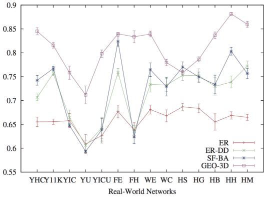
graphlets *agreement*

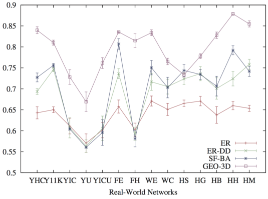
- *i-th orbit graphlet agreement* A_i [Prž07] defined as
  - $\widetilde{p}^i_k$ is *i-th orbit graphlet degree distribution* of *first network*
  - $\widetilde{q}^i_k$ is *i-th orbit graphlet degree distribution* of *second network*

$$A_i = 1 - \sqrt{\tfrac{1}{2} \textstyle\sum_k \left(\log \widetilde{q}^i_k - \log \widetilde{p}^i_k\right)^2}$$

- *arithmetic/geometric graphlet agreement* A defined as

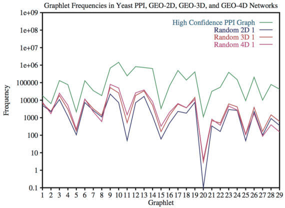
$$A = \tfrac{1}{73} \textstyle\sum_i A_i \qquad\qquad A = \left(\textstyle\prod_i A_i\right)^{\frac{1}{73}}$$



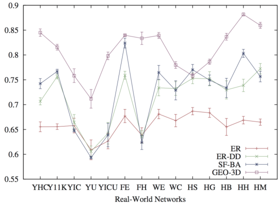


arithmetic/geometric graphlet agreement of protein networks and random graphs

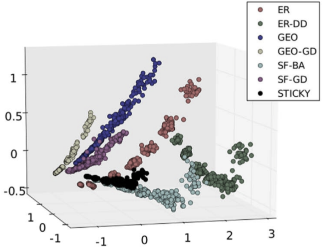
graphlets *overview*

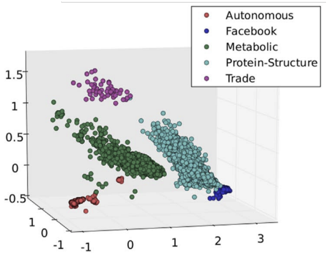


relative graphlet frequency [PCJ04]



graphlet distribution agreement [Prž07]





graphlet correlation matrix and *distance* [YMDD+14]

fragments *references*

Toby Davies and Elio Marchione.
Event networks and the identification of crime pattern motifs.
PLoS ONE, 10(11):e0143638, 2015.

Ernesto Estrada and Philip A. Knight.
A First Course in Network Theory.
Oxford University Press, 2015.

Tomaž Hočevar and Janez Demšar.
A combinatorial approach to graphlet counting.
Bioinformatics, 30(4):559–565, 2014.

Ron Milo, Shalev Itzkovitz, Nadav Kashtan, Reuven Levitt, Shai Shen-Orr, Inbal Ayzenshtat, Michal Sheffer, and Uri Alon.
Superfamilies of evolved and designed networks.
Science, 303(5663):1538–1542, 2004.

R. Milo, S. Shen-Orr, S. Itzkovitz, N. Kashtan, D. Chklovskii, and U. Alon.
Network motifs: Simple building blocks of complex networks.
Science, 298(5594):824–827, 2002.

N. Pržulj, D. G. Corneil, and I. Jurisica.
Modeling interactome: Scale-free or geometric?
Bioinformatics, 20(18):3508–3515, 2004.

Nataša Pržulj.
Biological network comparison using graphlet degree distribution.
Bioinformatics, 23(2):e177–e183, 2007.

fragments *references*

Sergi Valverde and Ricard V. Solé.
Network motifs in computational graphs: A case study in software architecture.
Phys. Rev. E, 72(2):026107, 2005.

Ömer Nebil Yaveroğlu, Noël Malod-Dognin, Darren Davis, Zoran Levnajić, Vuk Janjic, Rasa Karapandza, Aleksandar Stojmirovic, and Nataša Pržulj.
Revealing the hidden language of complex networks.
Sci. Rep., 4:4547, 2014.