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Turing-Roche knowledge event

Anthony Baptista

27/02/2024

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Introduction

Statistical physics of liquids

SORBONNE UNIVERSITÉS

LPTMC

Theoretical model for complex disorder

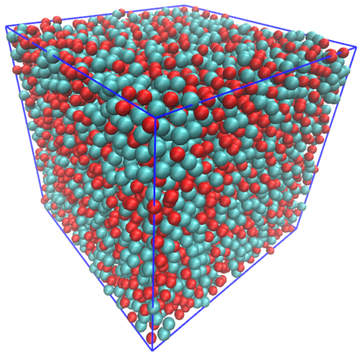
$$g_{ab}(r) = e^{-\beta v_{ab}(r) + h_{ab}(r) - c_{ab}(r) + b_{ab}(r)}$$

$$b_{ab}(r) = b_{ab}^{(CD)}(r) + b_{ab}^{(SD)}(r)$$

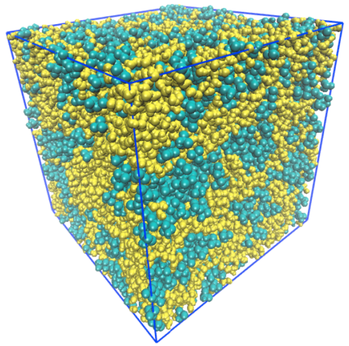
$$b_{ab}^{(CD)}(r) = \epsilon_1 \exp\left[-(r-\alpha_1)^2/\kappa_1^2\right] - \epsilon_2 \exp\left[-(r-\alpha_2)^2/\kappa_2^2\right]$$

$$b_{ab}(r) = \sum_{m\geq 3} \frac{1}{m!} \sum_{k\geq 3}^{m} \frac{1}{k!} \sum_{\alpha_1 \ldots \alpha_k} \left(\prod_{l=1}^{k} \rho_{\alpha_l}\right) \int d\vec{r}_{13} \int d\vec{r}_{14} \ldots \int d\vec{r}_{1k} \left(\prod_{l=1}^{k} h_{a\alpha_k}(r_{1k})\right) c_{b\alpha_1 \ldots \alpha_n}^{(k+1)}(\vec{r}_2, \vec{r}_3, \ldots, \vec{r}_k)$$

Simulation based on molecular dynamics



Simple disorder



Complex disorder

AIP The Journal of Chemical Physics

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Home > The Journal of Chemical Physics > Volume 150, Issue 6 > 10.1063/1.5066598

PREV NEXT

No Access • Submitted: 16 October 2018 • Accepted: 26 January 2019 • Published Online: 13 February 2019

Modeling micro-heterogeneity in mixtures: The role of many body correlations

J. Chem. Phys. **150**, 064504 (2019); https://doi.org/10.1063/1.5066598

Anthony Baptista *and* Aurélien Perera

Issue 18, 2019

Previous Article Next Article

From the journal:
Physical Chemistry Chemical Physics

Microscopic origin of the scattering pre-peak in aqueous propylamine mixtures: X-ray and neutron experiments *versus* simulations

Check for updates

László Almásy, [ab] Alexander I. Kuklin, [c] Martina Požar, [d] Anthony Baptista [e] and Aurélien Perera [*e]

Network theory for biology

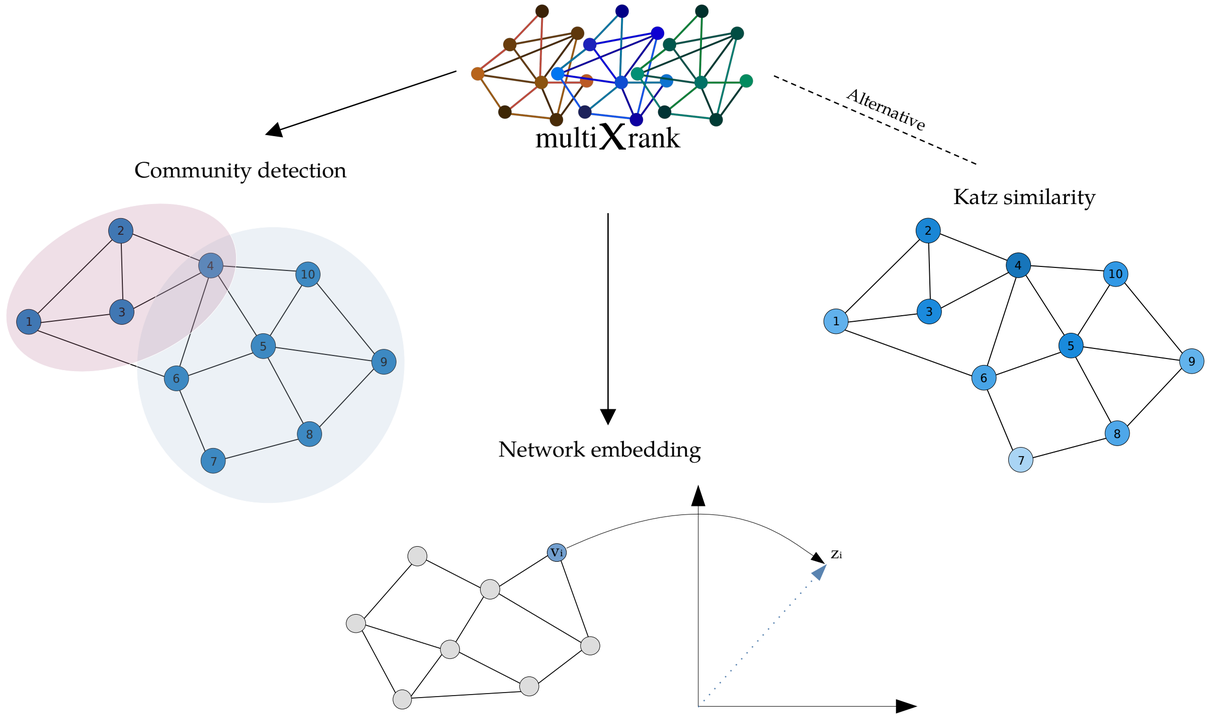
Marseille Medical Genetics

CENTURI
TURING CENTRE FOR LIVING SYSTEMS

Article | Open Access | Published: 01 July 2022

Universal multilayer network exploration by random walk with restart

Anthony Baptista, Aitor Gonzalez & Anaïs Baudot



RESEARCH

Random Walk with Restart on multilayer networks: from node prioritisation to supervised link prediction and beyond

Anthony Baptista[1,2*], Galadriel Brière[3] and Anaïs Baudot[4,5*]

TOPICAL REVIEW • OPEN ACCESS

Zoo guide to network embedding

A Baptista[8,1,2], R J Sánchez-García[2,3,4], A Baudot[5,6,7] and G Bianconi[8,1,2]

The molecular landscape of premature aging diseases defined by multilayer network exploration

Cécile Beust[1,2,†], Alberto Valdeolivas[1,3,†], Anthony Baptista[1,4,5], Galadriel Brière[1,6], Nicolas Lévy[1,7], Ozan Ozisik[1,8], and Anaïs Baudot[1,9,10]

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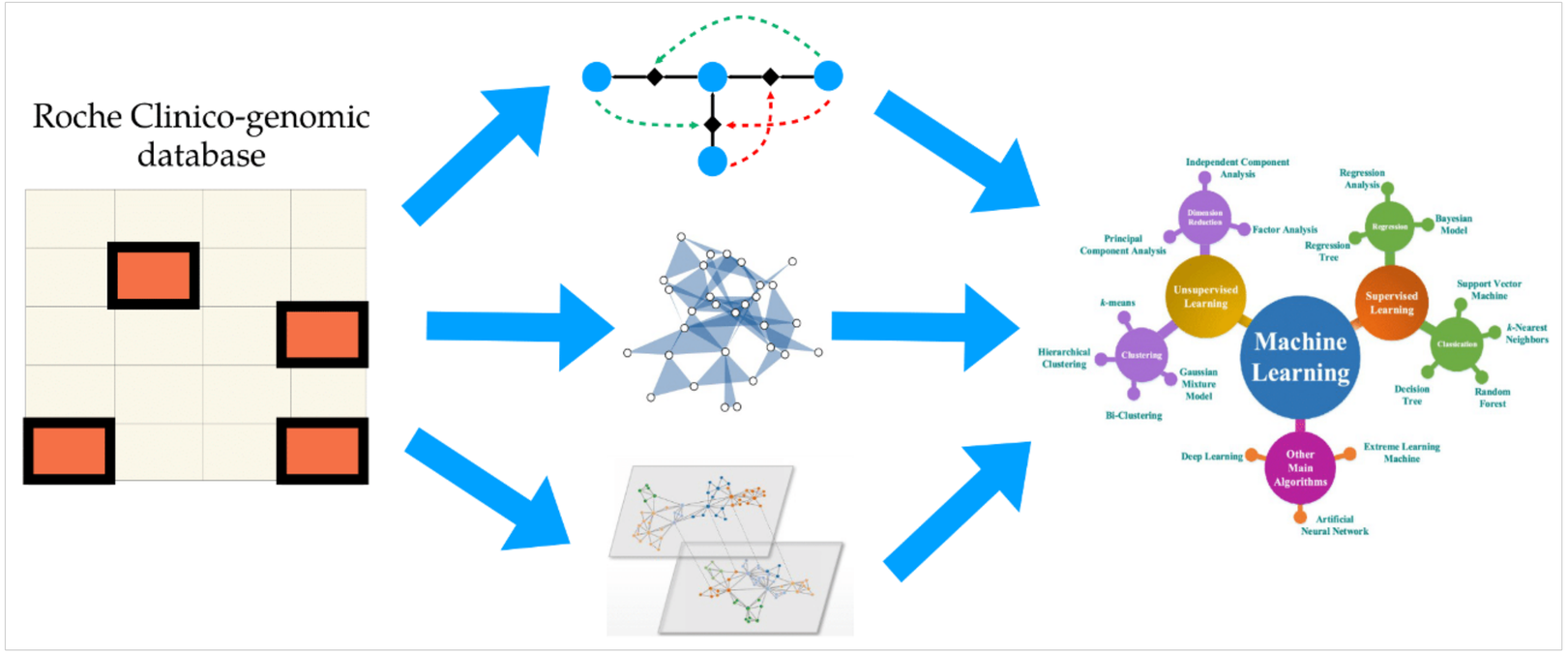
Using network science to quantify the geometry of "missingness"



1. Characterize pairwise and higher-order interactions
2. Extract Structural Missingness Networks (SMNs)
3. Characterize the Geometry of SMNs

Professor Ginestra Bianconi

Dr Ruben Sanchez Garcia

Dr Anthony Baptista

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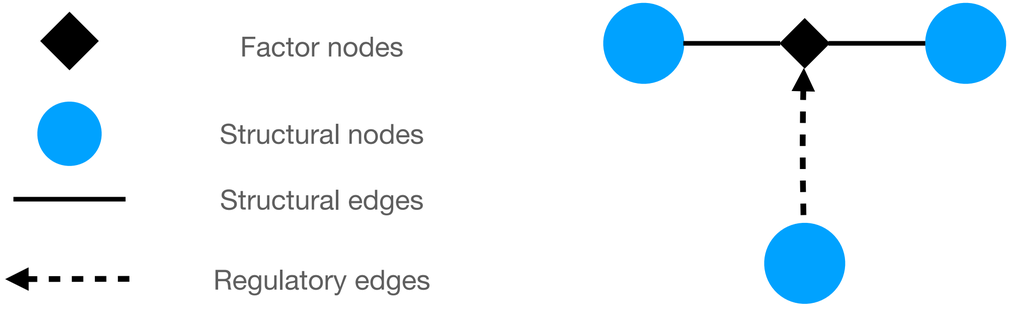
Triadic interactions

Triadic interactions

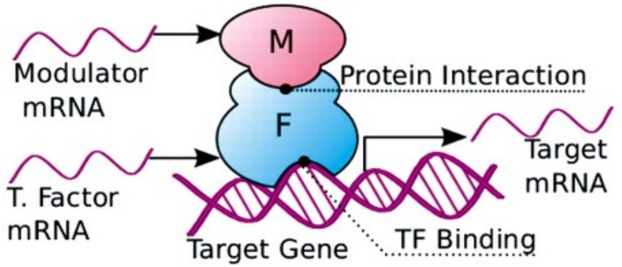
Triadic interactions in both continuous and discrete real data

The structural network $G_S = (V, E_S)$
* N nodes
* L edges

The regulatory network (bipartite)
$G_R = (V, E_S, E_R)$
* Nodes given by V
* Nodes given by E_S
* Both types of nodes connected by the regulatory interactions E_R ($|E_R| = \hat{L}$).

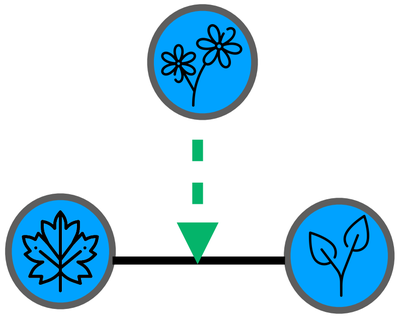


Gene regulatory network



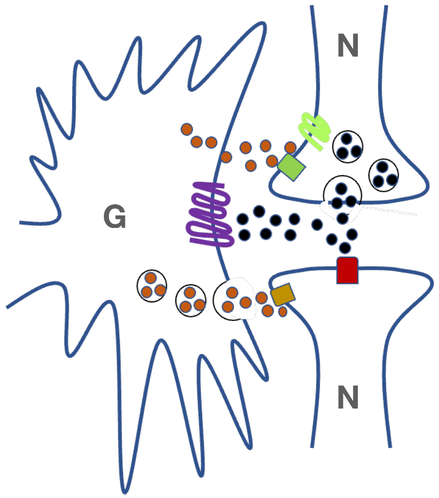
Wang, K. et al., Nat Biotechnol (2009)

Ecological network



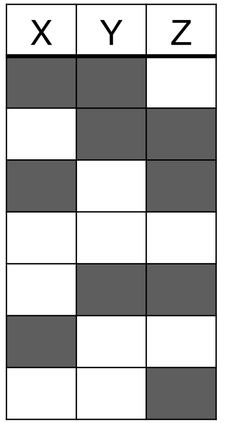
Grilli, J. *et al., Nature* (2017)
Bairey, E. Et al., *Nat Commun* (2016)

Neurological network



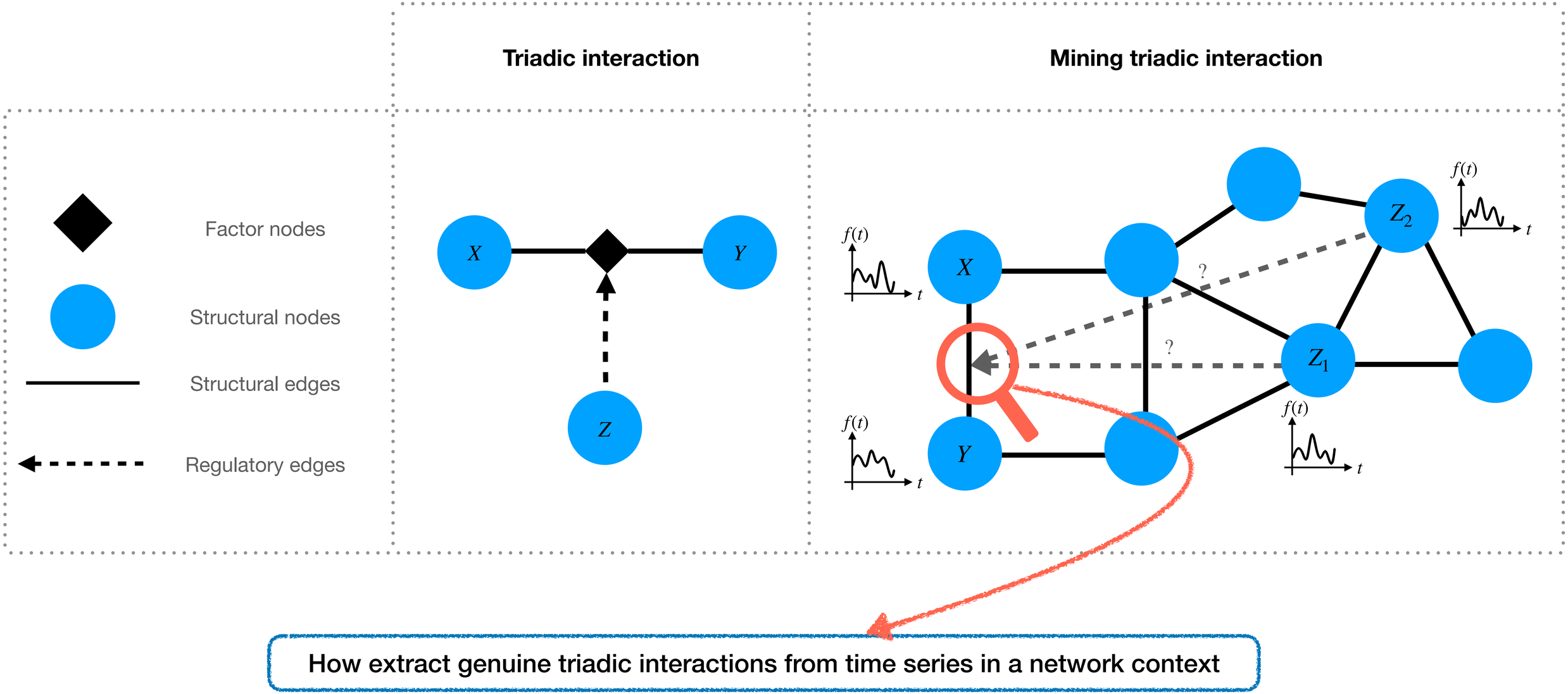
Woo-Hyun C. *et al., Exp Neurobiol (2016)*

Structured missingness



Mitra, R., McGough, S.F., Chakraborti, T. *et al. Nat Mach Intell* (2023)

Mining triadic interactions



How extract genuine triadic interactions from time series in a network context

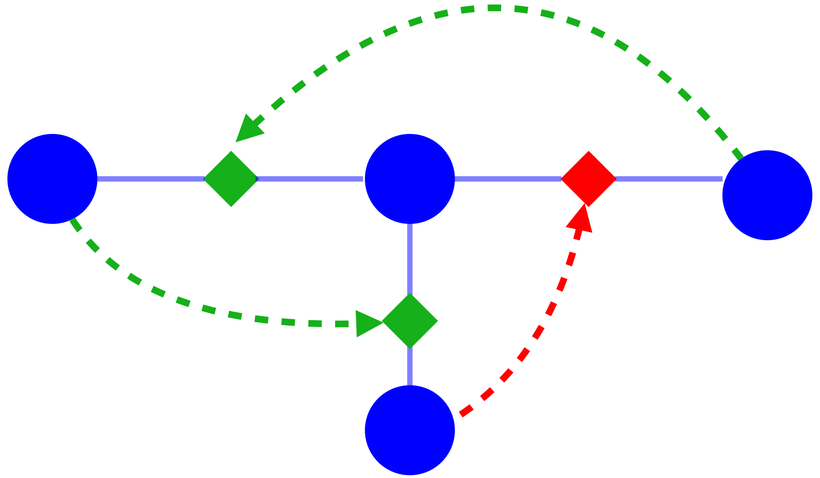
Strength and sign of triadic interaction

Mutual information (given Z = z)

$$MI(X,Y\,|\,Z=z)=\sum_{x,y}p(x,y\,|\,z)\ln\frac{p(x,y\,|\,z)}{p(x\,|\,z)p(y\,|\,z)}$$

Conditional Mutual Information

$$MI_{X,Y;Z}=\langle MI(X,Y\,|\,Z=z)\rangle=\sum_{z}p(z)MI(X,Y\,|\,Z=z)$$



Strength of triadic interaction

$$\Sigma_{X,Y;Z}=\sqrt{\sum_{z}p(z)\left[MI(X,Y\,|\,Z=z)-MI_{X,Y;Z}\right]^2}>0$$

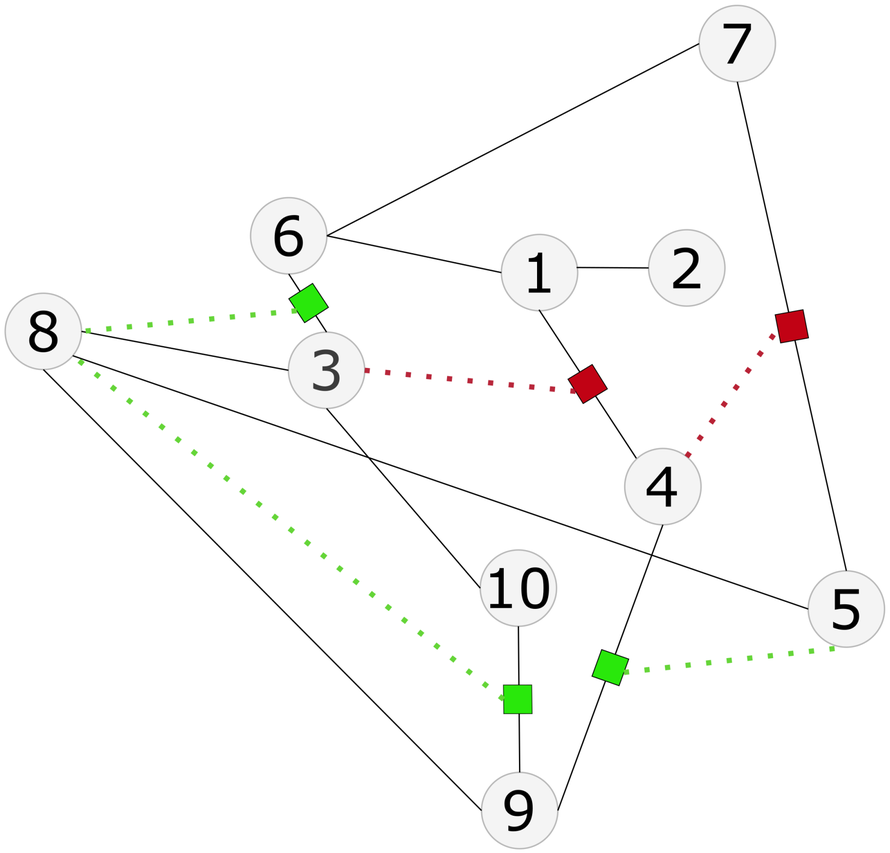
$$T_{X,Y;Z}=\max_{z}\left|MI(X,Y\,|\,Z=z)-MI_{X,Y;Z}\right|>0$$

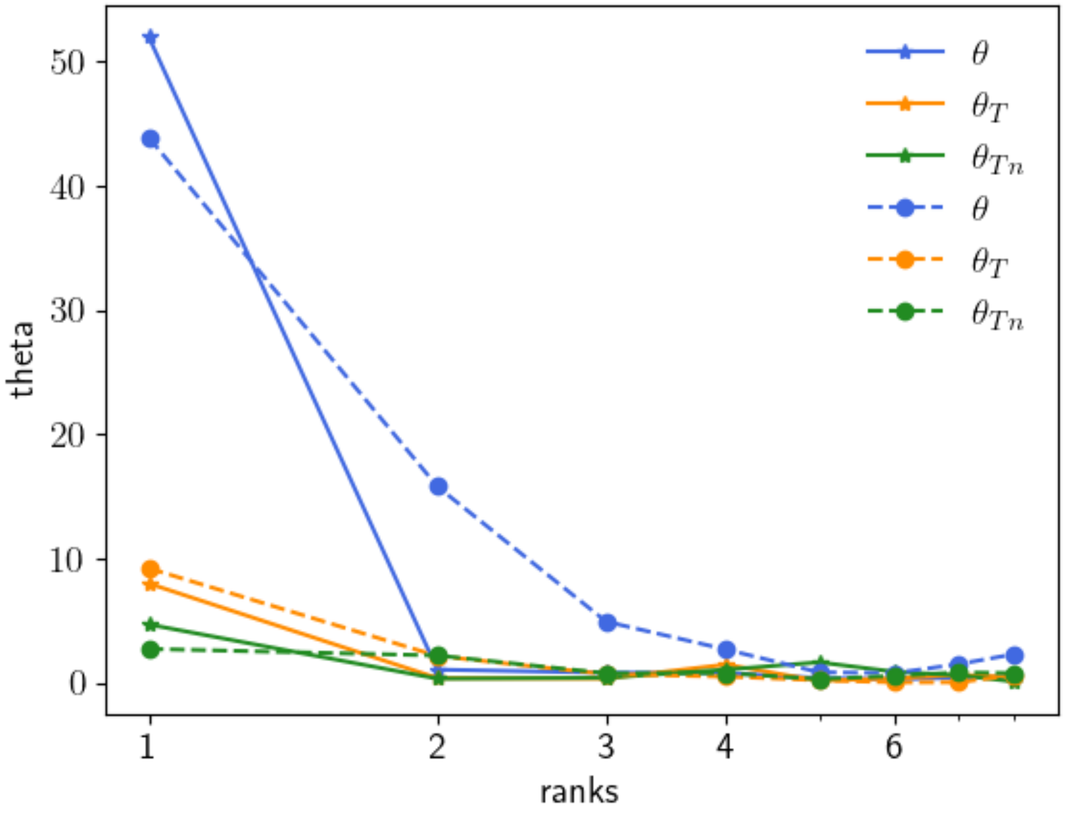
$$T_{nX,Y;Z}=\max_{z}\left|MI(X,Y\,|\,Z=z)-MI(X,Y\,|\,Z=z+\Delta z)\right|>0$$

Sign of triadic interaction

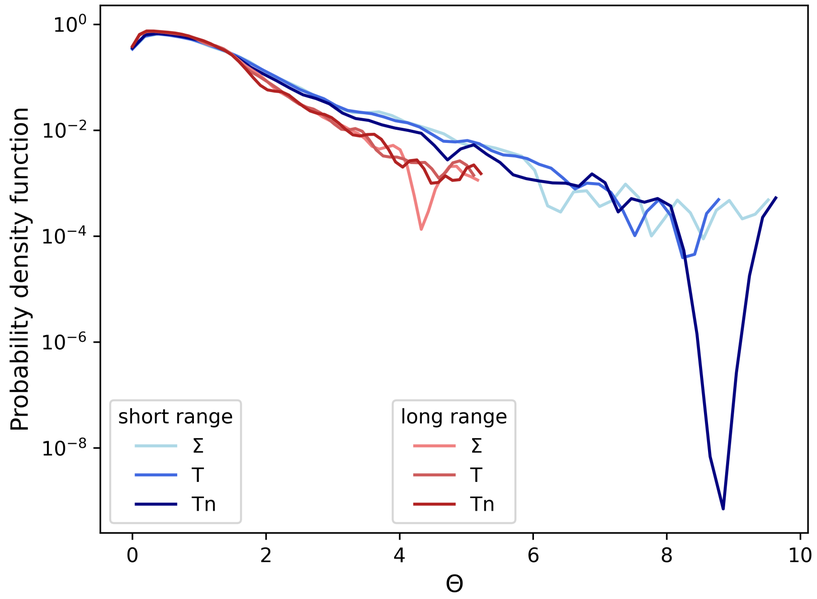
$$C=\frac{\langle zMI(X,Y\,|\,Z=z)\rangle-\langle z\rangle\langle MI(X,Y\,|\,Z=z)\rangle}{\sigma_z\sigma_{MI}}$$

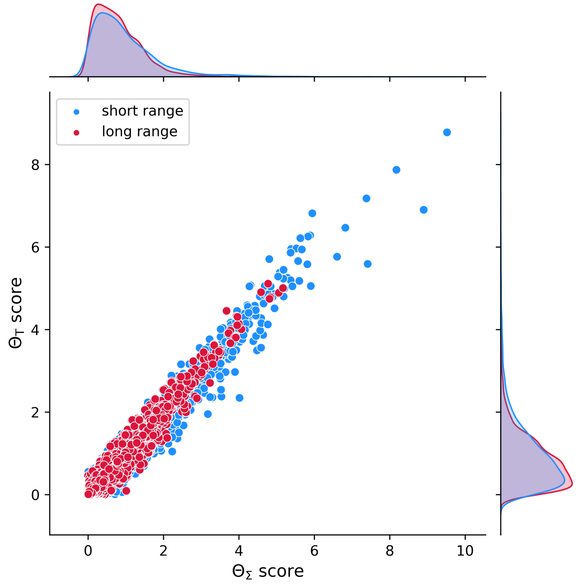
Toy model

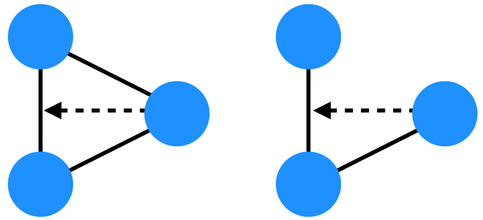

7
6
1
2
8
3
4
10
5
9

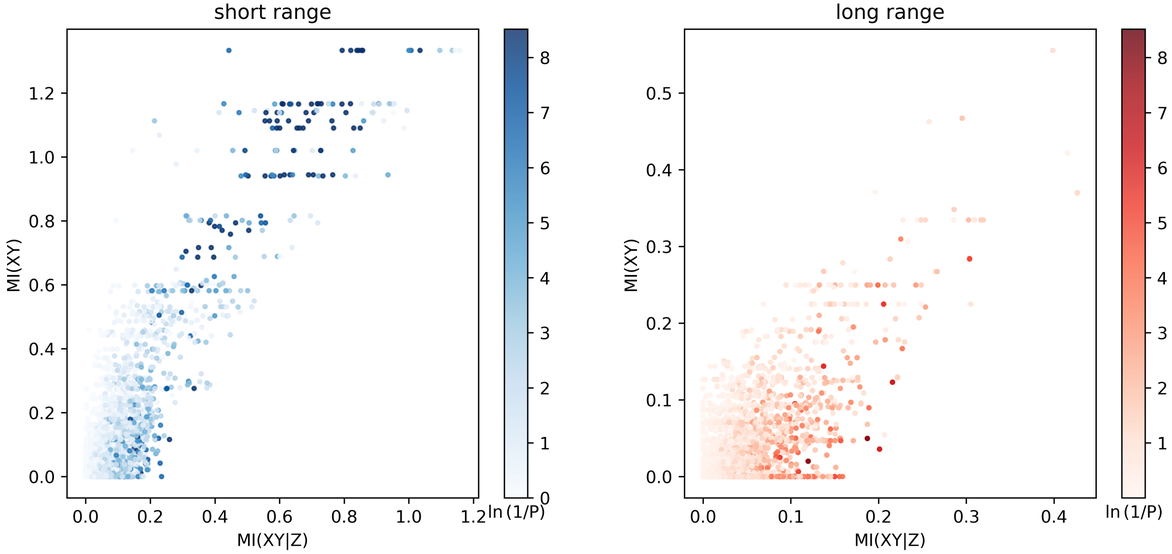

50
40
30
20
10
0
theta
1
2
3
4
6
ranks
θ
θ_T
θ_{Tn}
θ
θ_T
θ_{Tn}

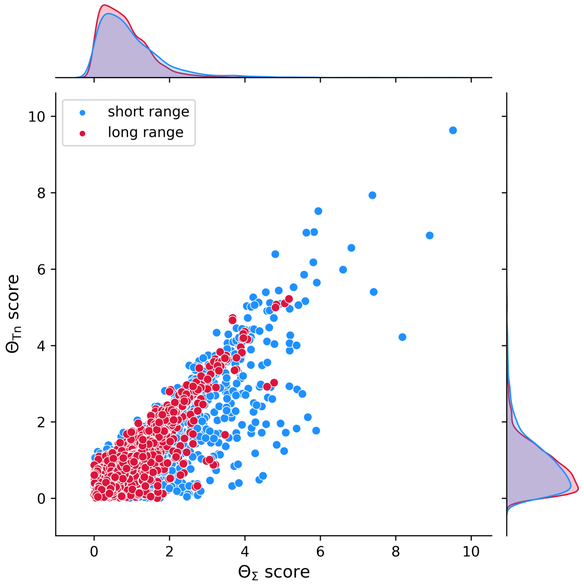
Comparison of measures to detect triadic interactions

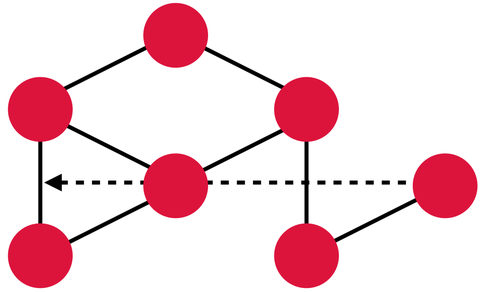




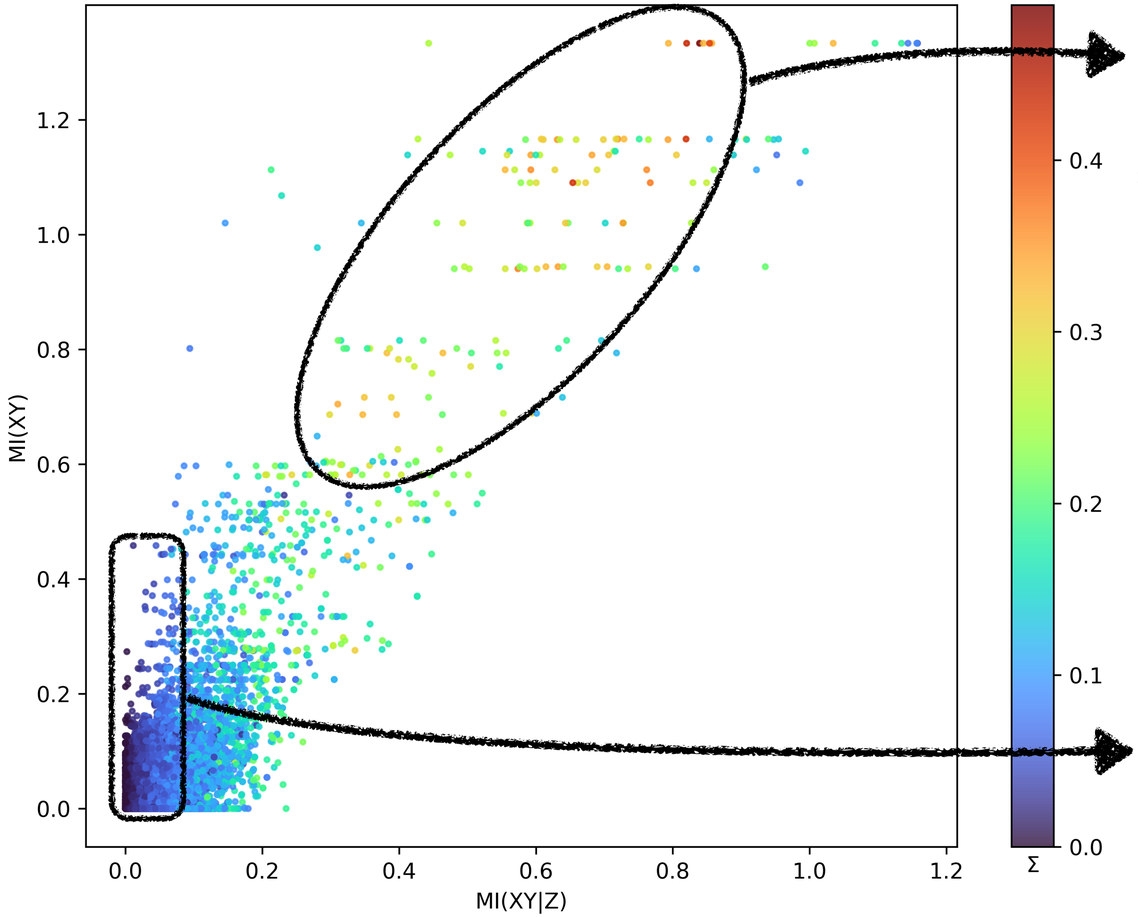


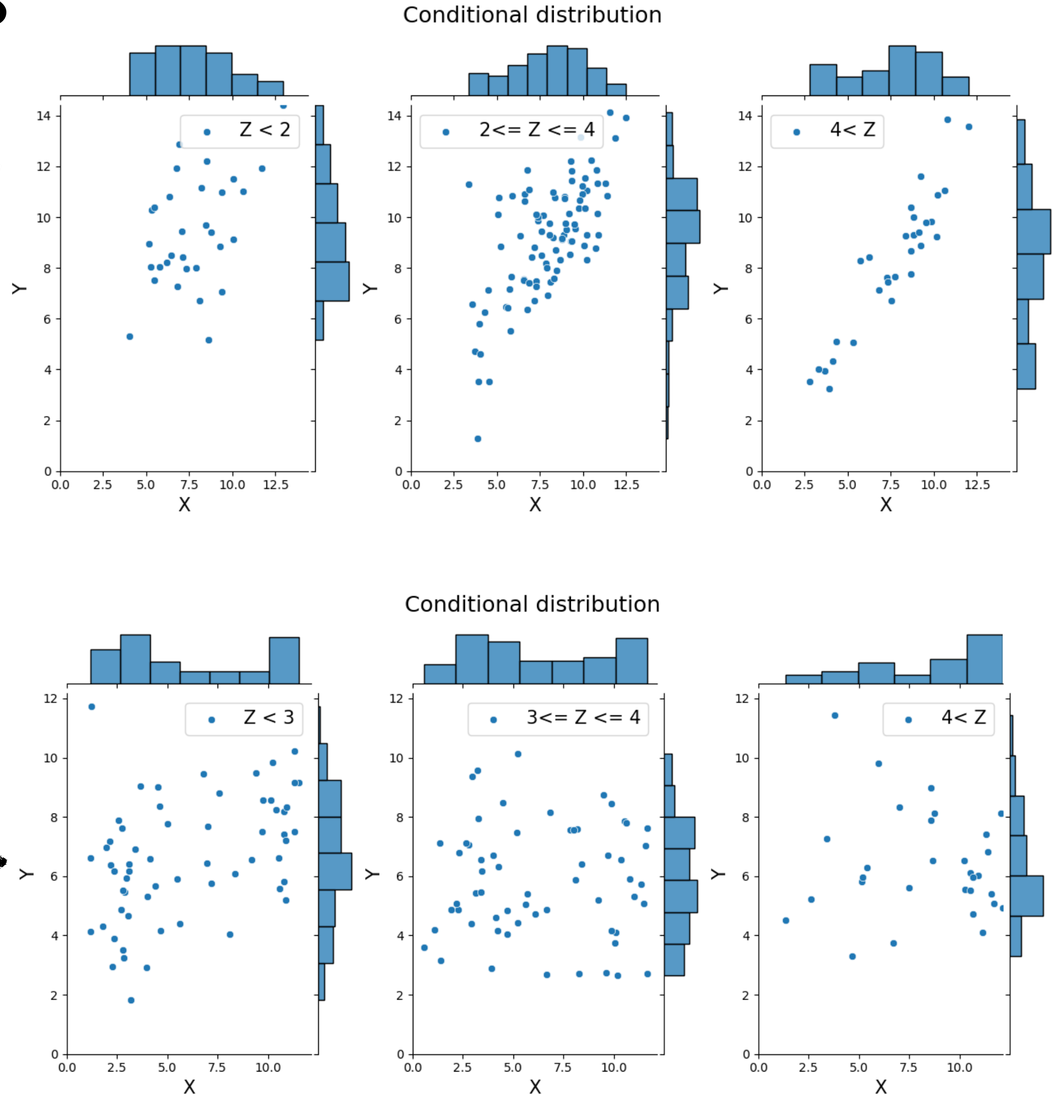






Detection of triadic interactions

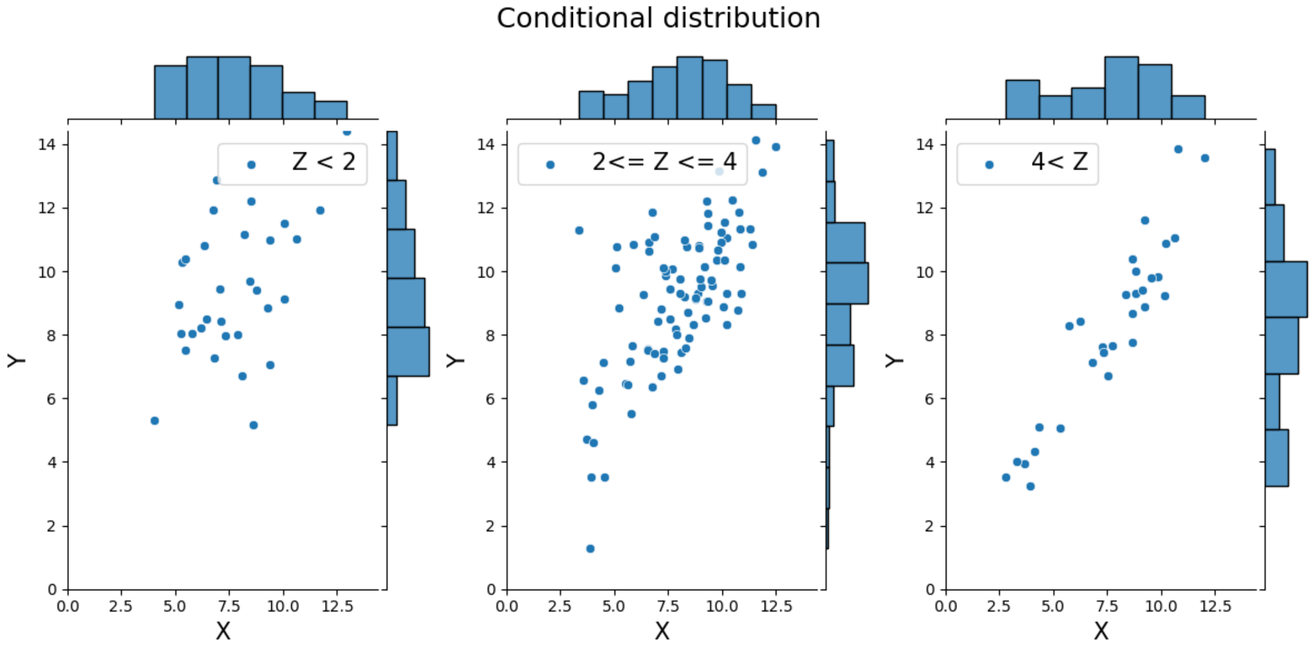


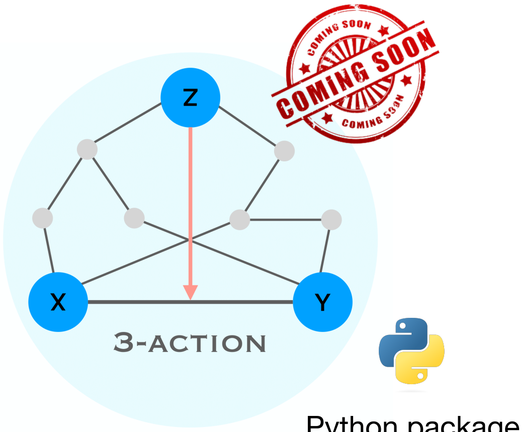


$$\Sigma_{X,Y;Z} = \sqrt{\langle (MI(X,Y \mid Z=z) - I(X,Y \mid Z))^2 \rangle} > 0$$

Σ scores separate strong triadic interactions from non triadic interactions

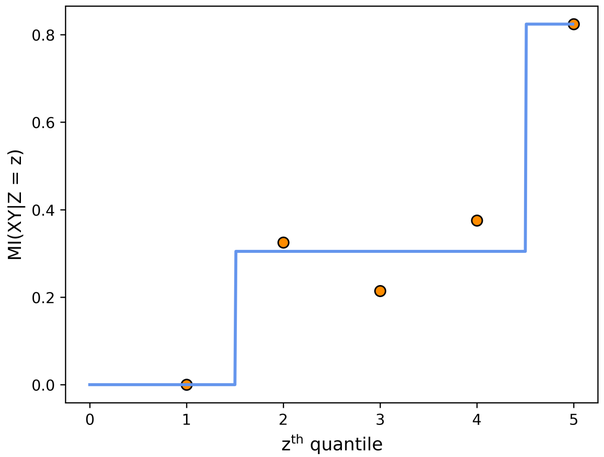
Detection of triadic interactions



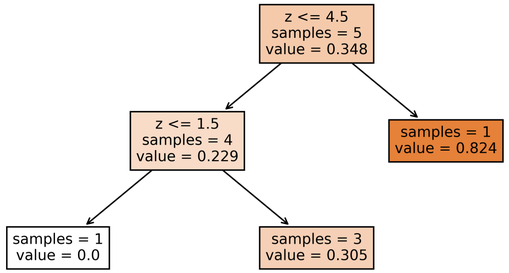


Python package

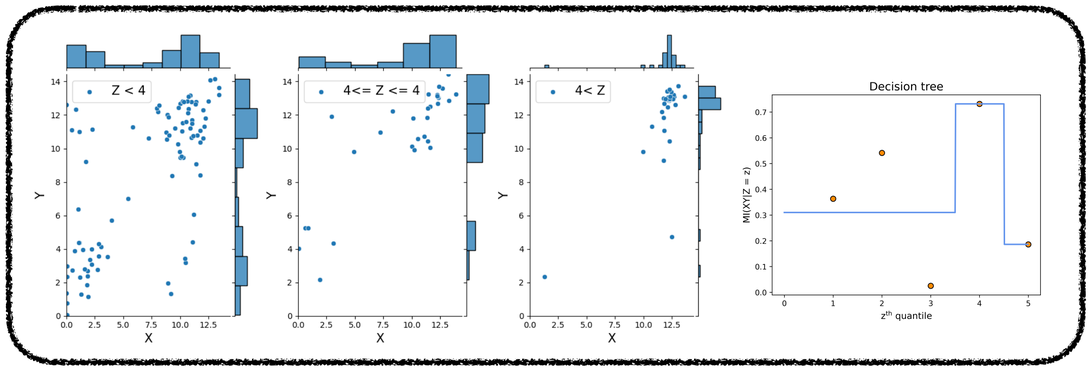
Regression plot



Decision tree

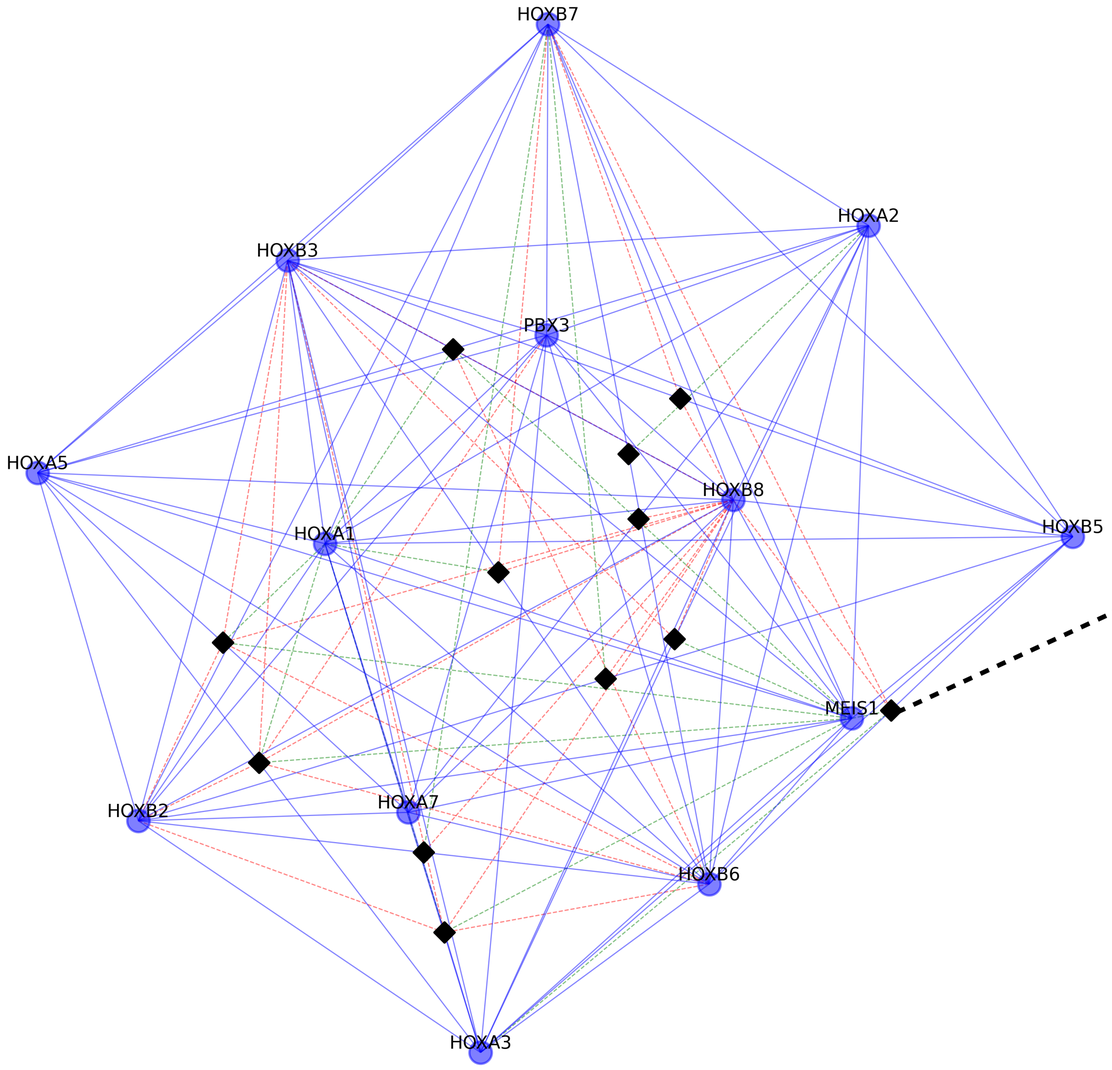


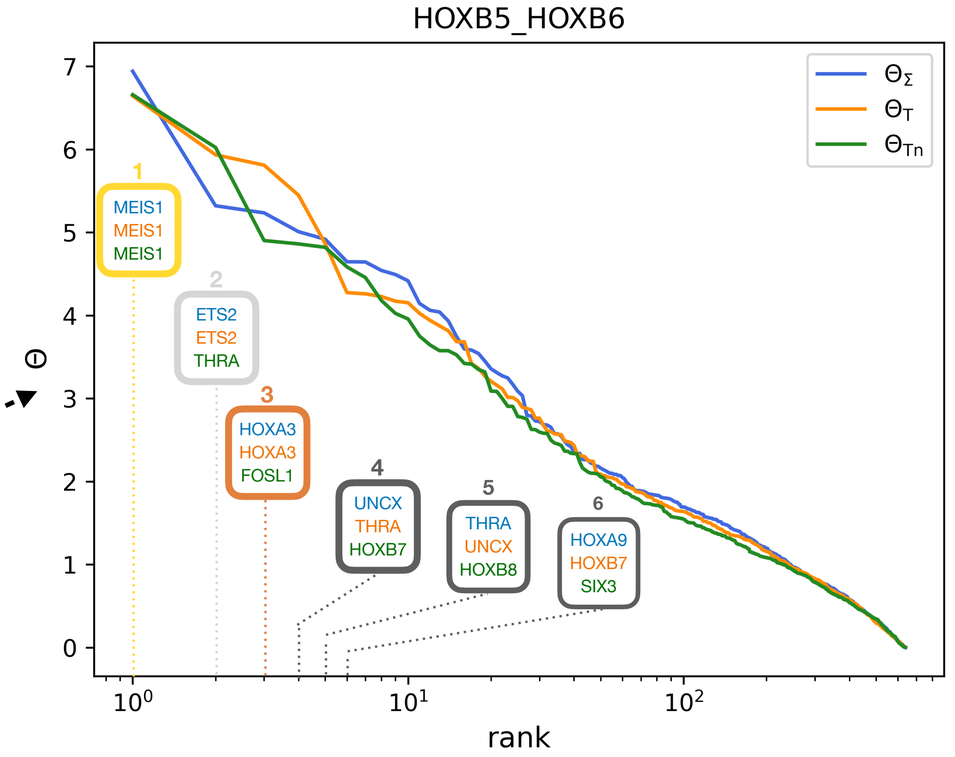
Non-monotonic



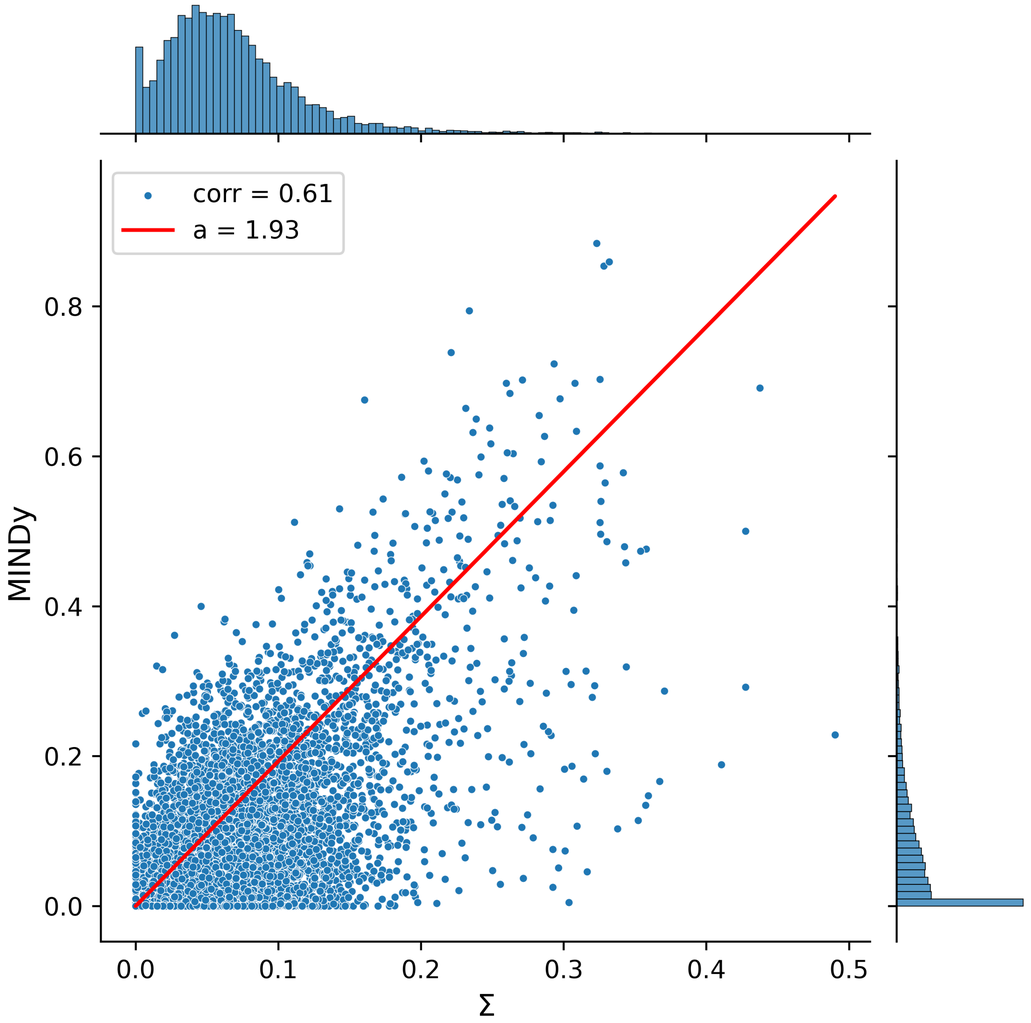
Triadic interaction network

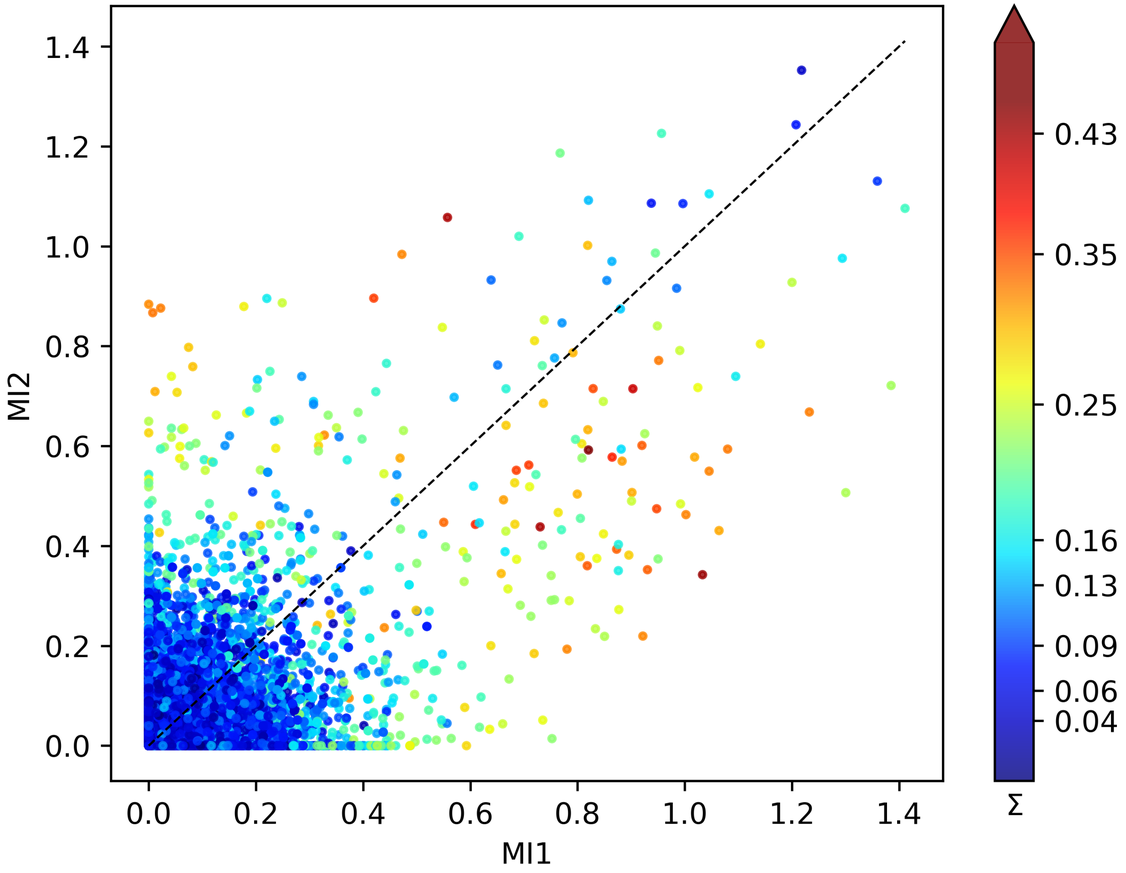
Acute Myeloid Leukemia gene expression





Comparison with former method (MINDy)

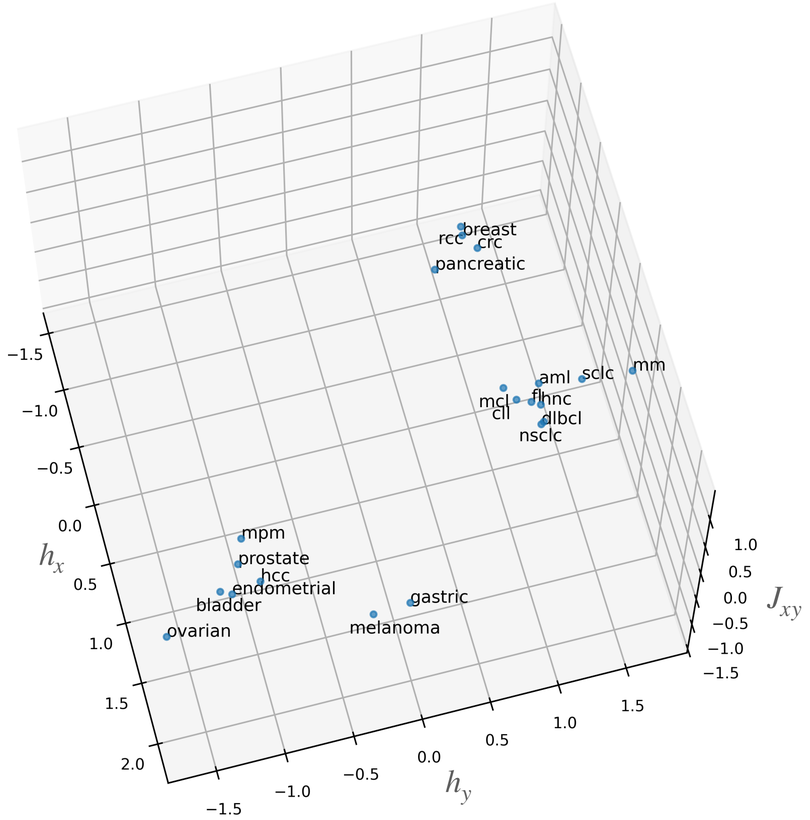




Detection of triadic interactions

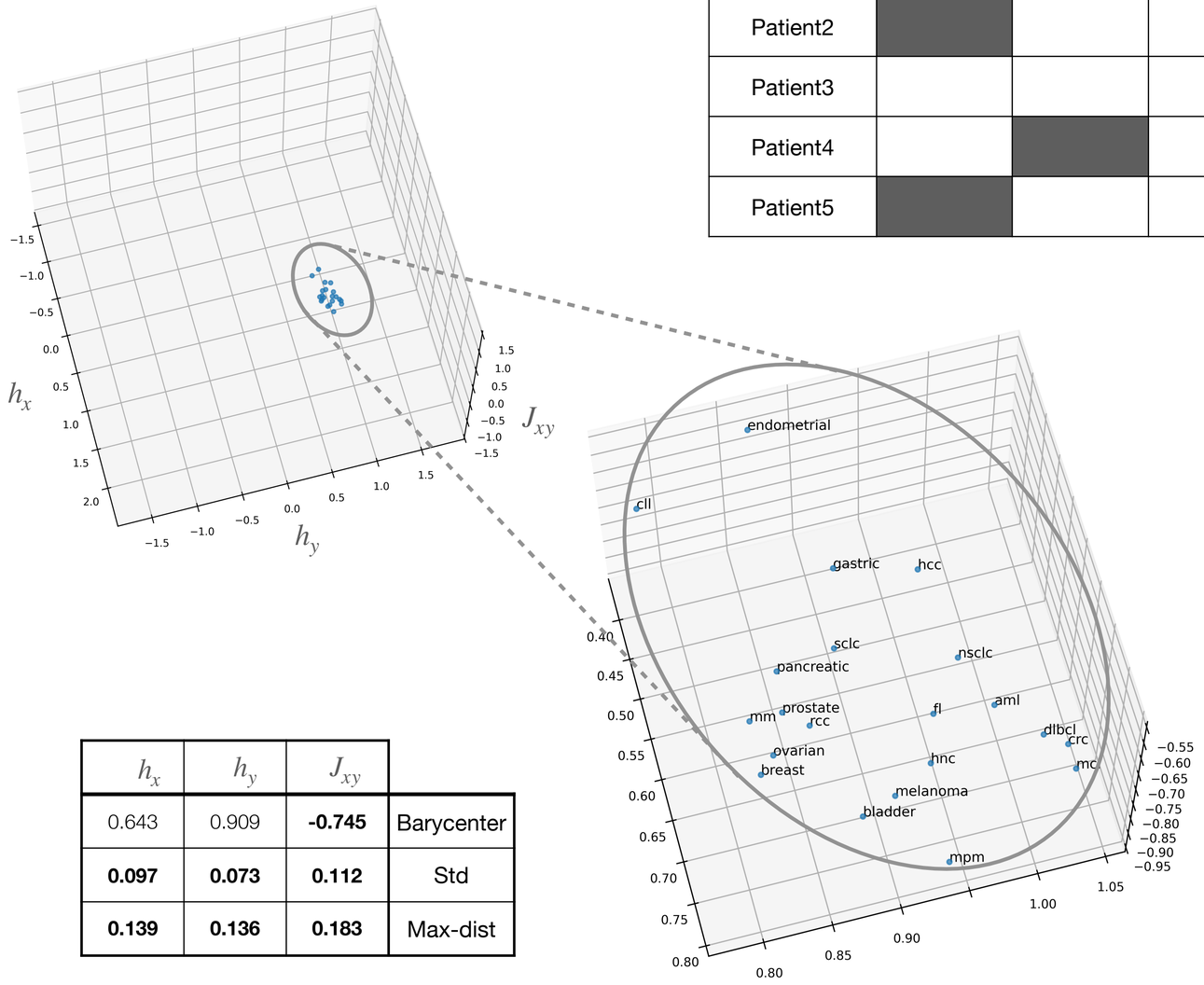
Structure missingness (bimodal variables)

Real data



	h_x	h_y	J_{xy}
Barycenter	-0.780	0.379	**-0.023**
Std	**1.006**	**1.046**	**1.047**
Max-dist	**1.283**	**1.330**	**1.341**

Null model

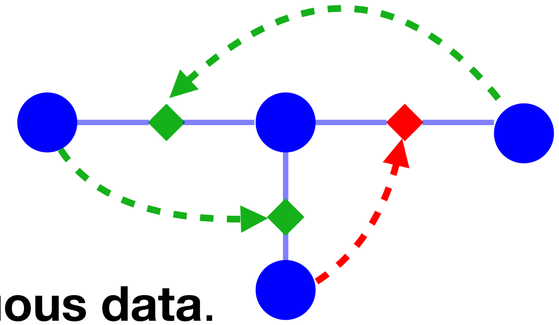


h_x	h_y	J_{xy}	
0.643	0.909	**-0.745**	Barycenter
0.097	**0.073**	**0.112**	Std
0.139	**0.136**	**0.183**	Max-dist

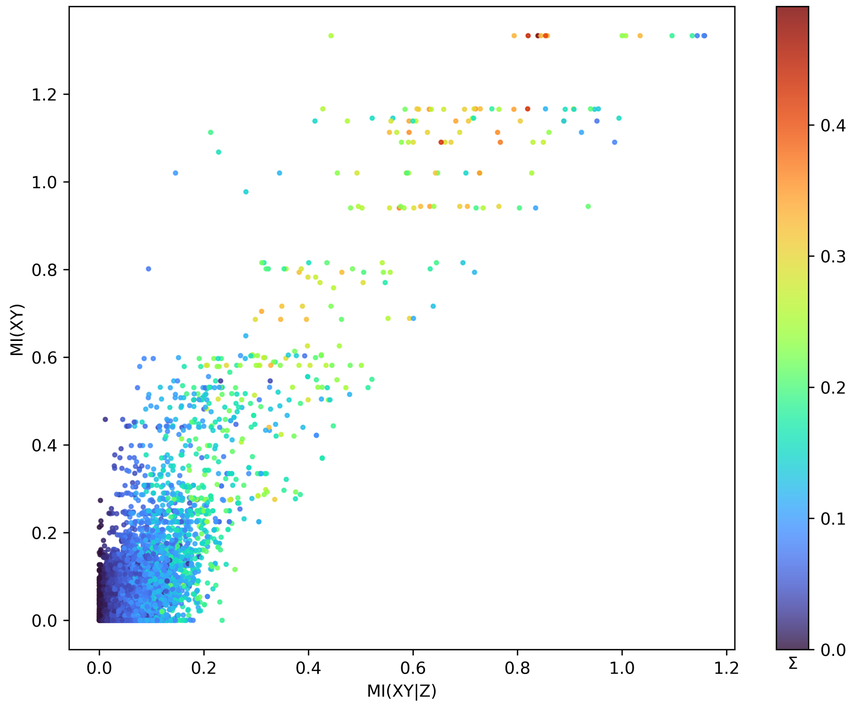
Indicator matrix

Role	X	Y	Z
Feature	Ismetastatic	tstage	Cancer type
Patient1			a
Patient2			a
Patient3			b
Patient4			b
Patient5			c

Conclusion

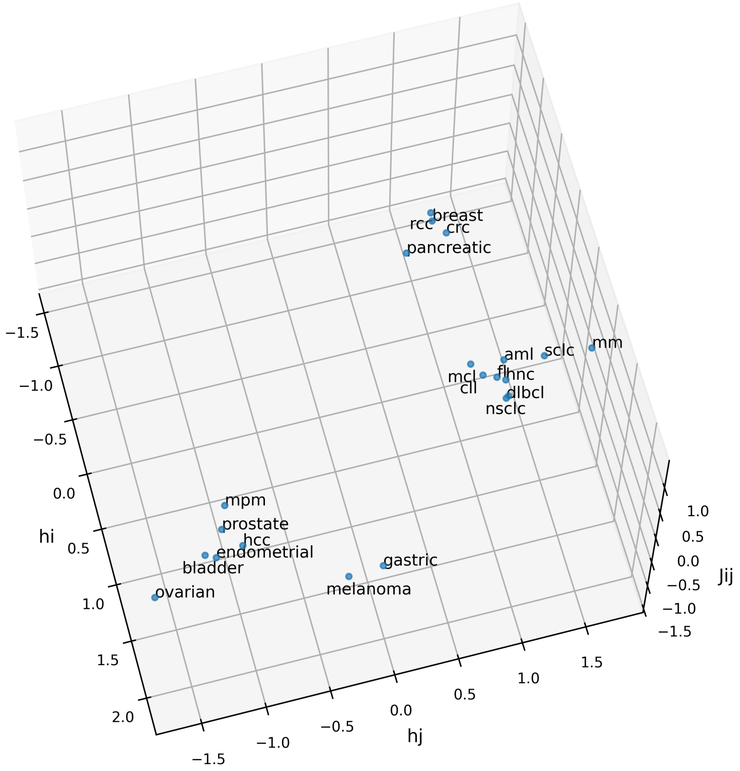


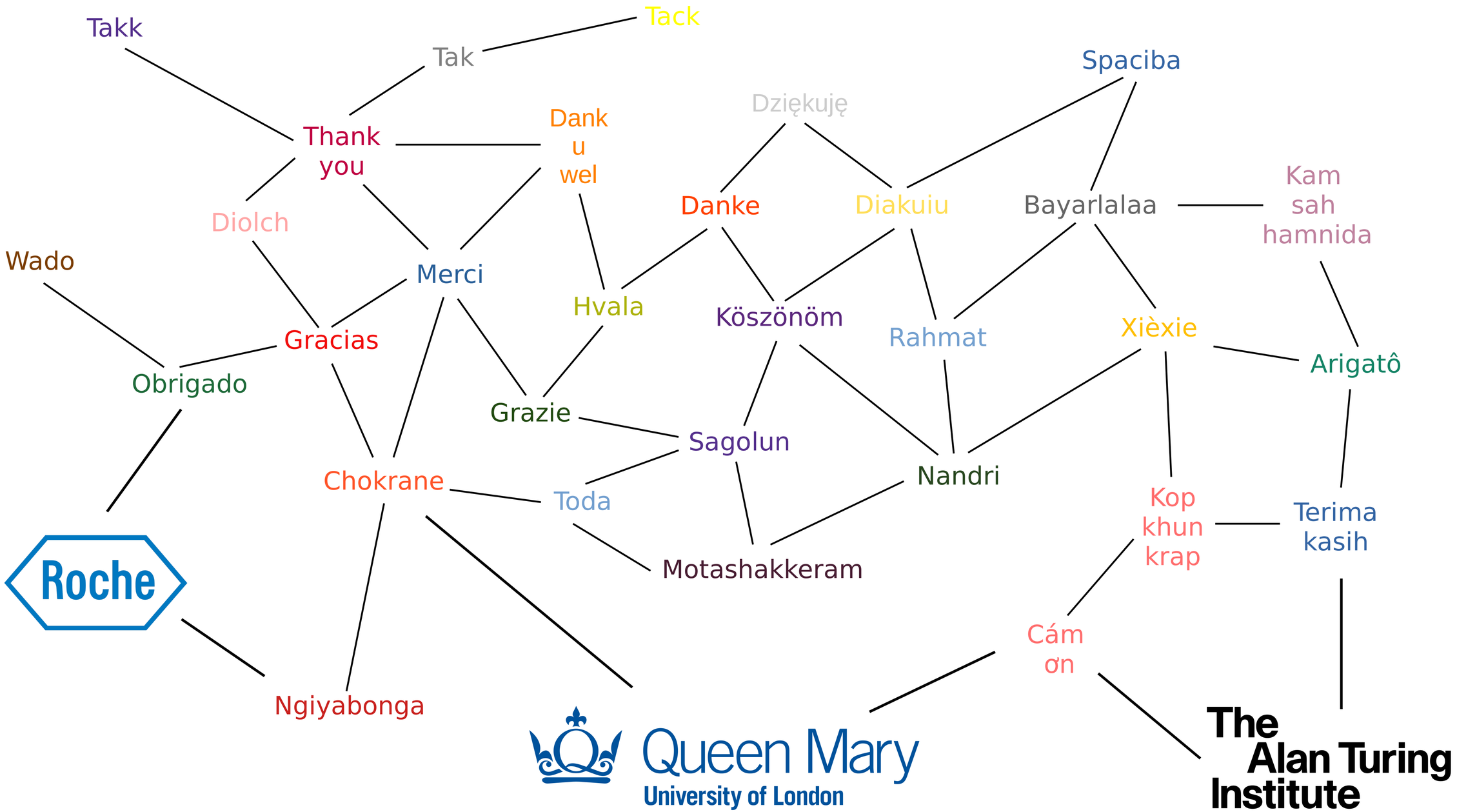
1. **Triadic interaction** manifests in **various systems**.
2. We have developed novel **measures** to identify triadic interactions in **continuous data**.
3. When dealing with **discrete data** (bimodal variables), we can quantitatively assess the intensity of triadic interactions.



Continuous data

Discrete data




Takk
Tack
Tak
Spaciba
Dziękuję
Thank you
Dank u wel
Danke
Diakuiu
Bayarlalaa
Kam sah hamnida
Diolch
Wado
Merci
Hvala
Köszönöm
Rahmat
Xièxie
Arigatô
Gracias
Obrigado
Grazie
Sagolun
Nandri
Chokrane
Toda
Kop khun krap
Terima kasih
Motashakkeram
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