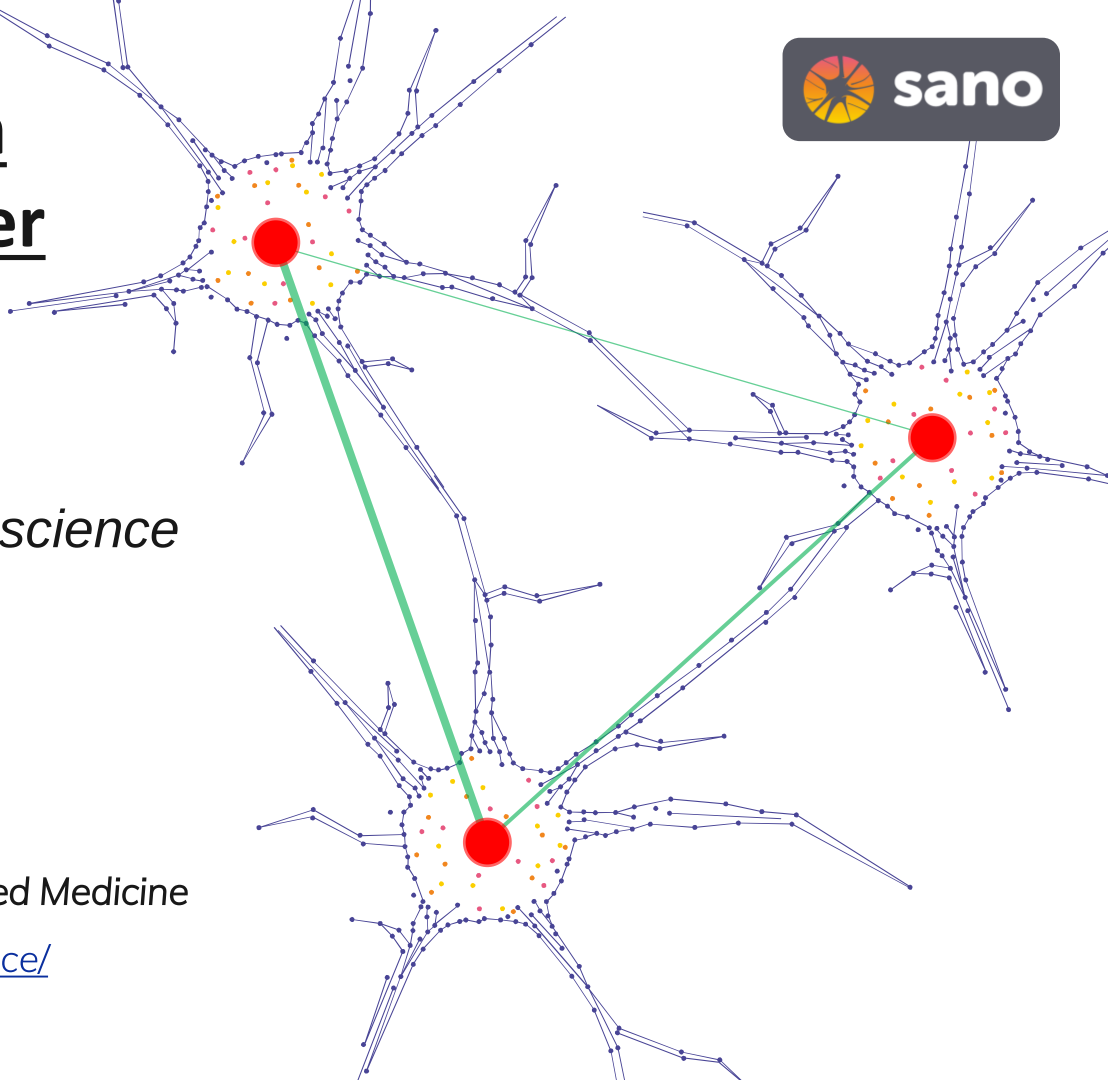
On the use of quantum technologies to discover brain structure and function

Applications to network (neuro)science



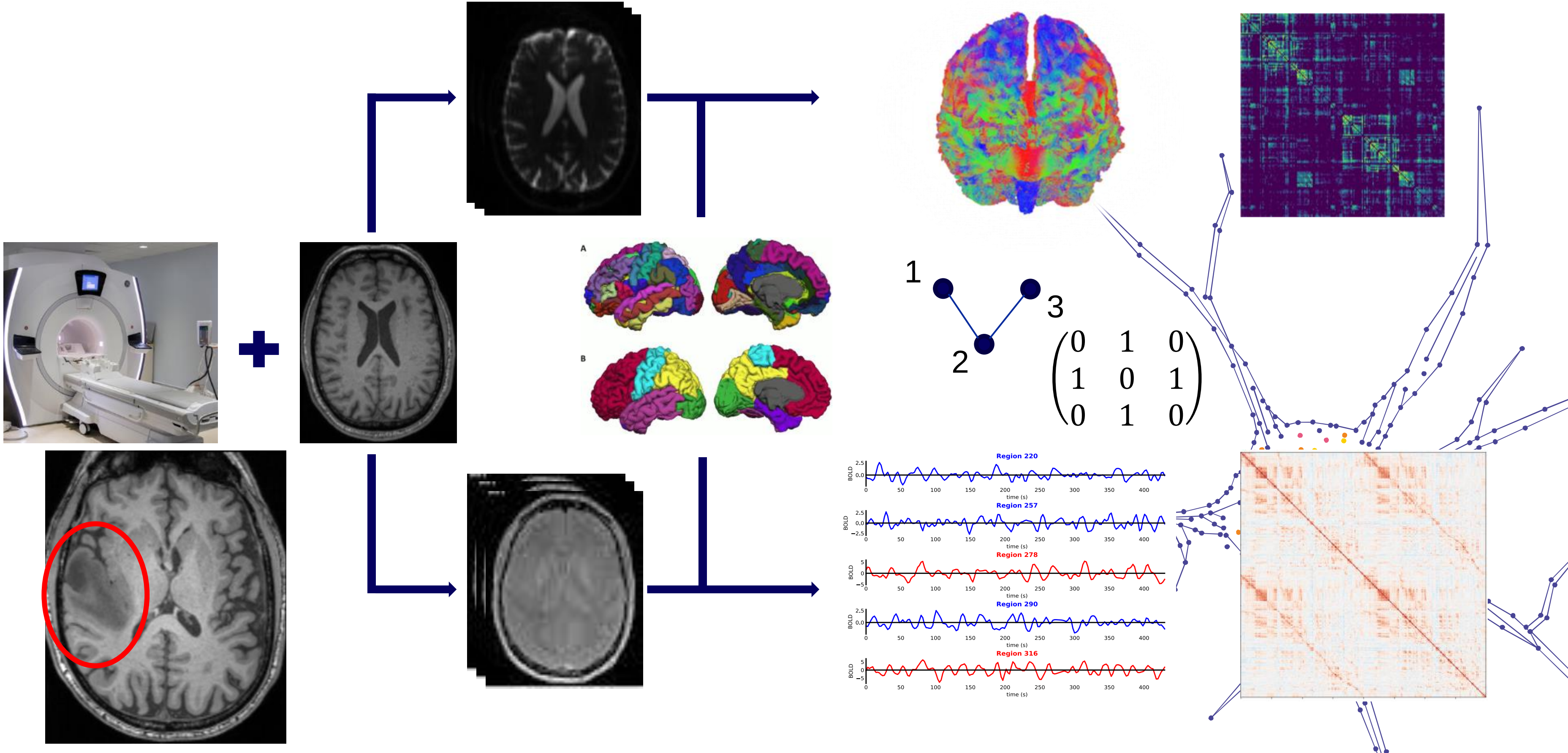
Joan Falcó-Roget

SANO - Center for Computation Personalised Medicine

Brain and More Lab https://bam.sano.science/

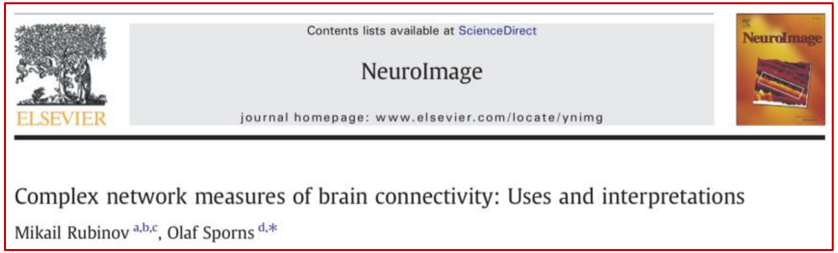
Network Neuroscience

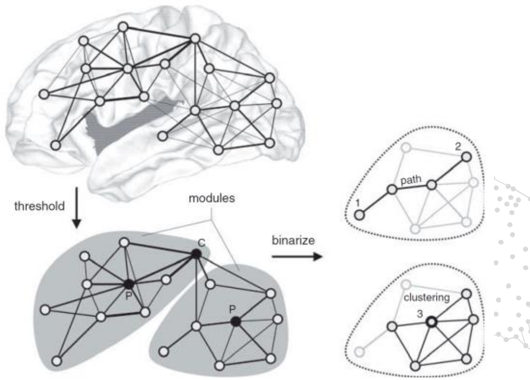
The brain as collections of *Graphs*

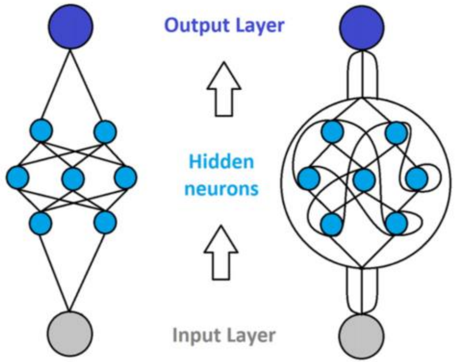


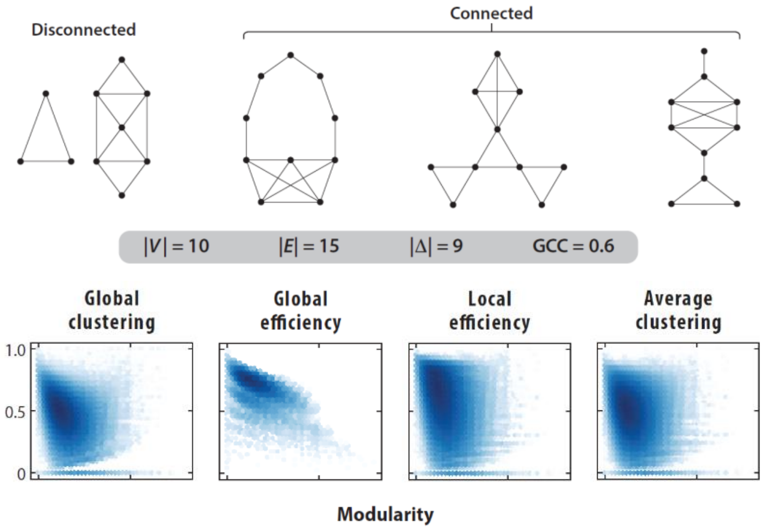
Network Neuroscience

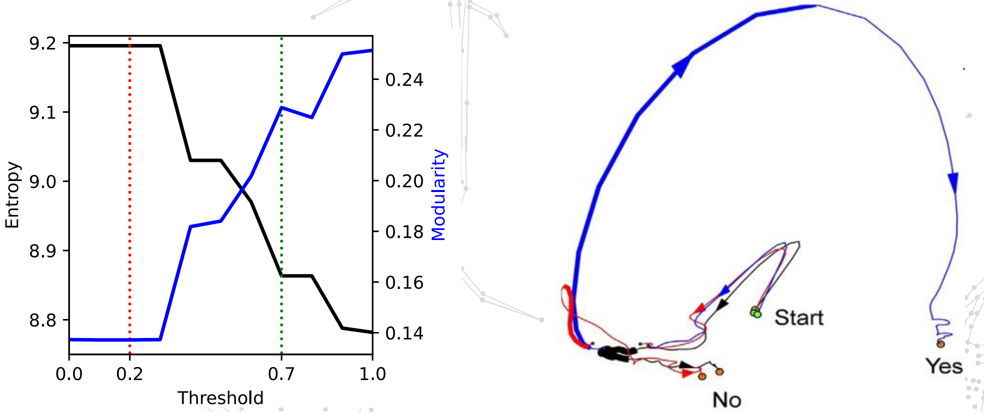
A wide range of numerical methods

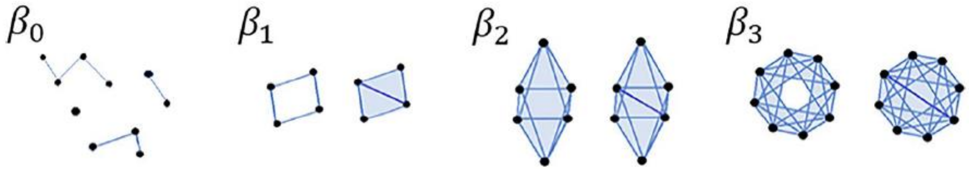












Rubinov & Sporns 2010; *Centeno*, et al. 2022; *Falcó-Roget*, et al. 2022; *Parga*, et al. 2023; *Chung*, et al. 2022; *Carnevale*, et al. 2015

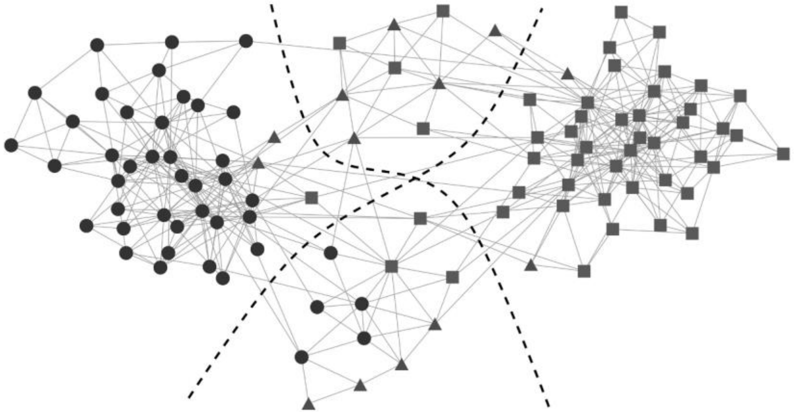
Modularity maximization

Discovering communities in Graphs and the Brain

$$Q = \sum_{s=1}^{k} \left[\frac{l_s}{m} - \gamma \left(\frac{d_s}{2m} \right)^2 \right]$$

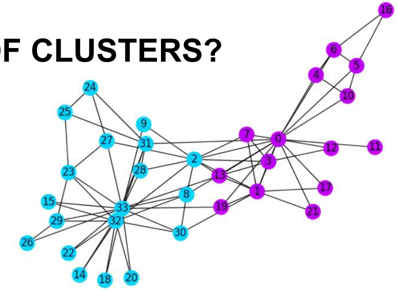
$$l_s = \sum_{i \in C_s} \sum_{j \in C_s} A_{ij}$$ Edges inside the cluster

$$d_s = \sum_{i \in C_s} g_i$$ Degrees of the nodes inside the cluster



WE DON'T KNOW THE NUMBER OF CLUSTERS?

$$\frac{1}{2}(s_i s_j + 1) \rightarrow 1, \; 0$$



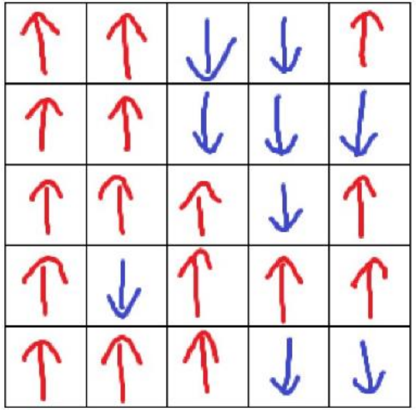
$$Q = \frac{1}{4m} \sum_{ij} \left(A_{ij} - \frac{g_i g_j}{2m} \right)(s_i s_j + 1) = \frac{1}{4m} \sum_{ij} \left(A_{ij} - \frac{g_i g_j}{2m} \right) s_i s_j$$

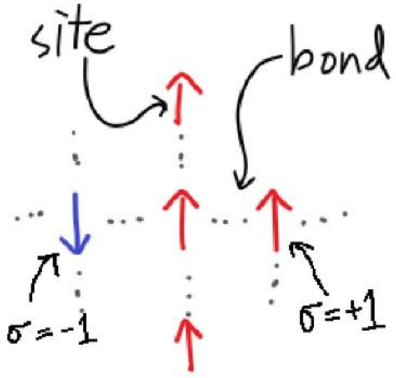
$$Q = \frac{1}{2m} \sum_{ij} B_{ij} \delta(c_i, c_j)$$ with $B_{ij} = A_{ij} - \frac{g_i g_j}{2m}$ the modularity matrix

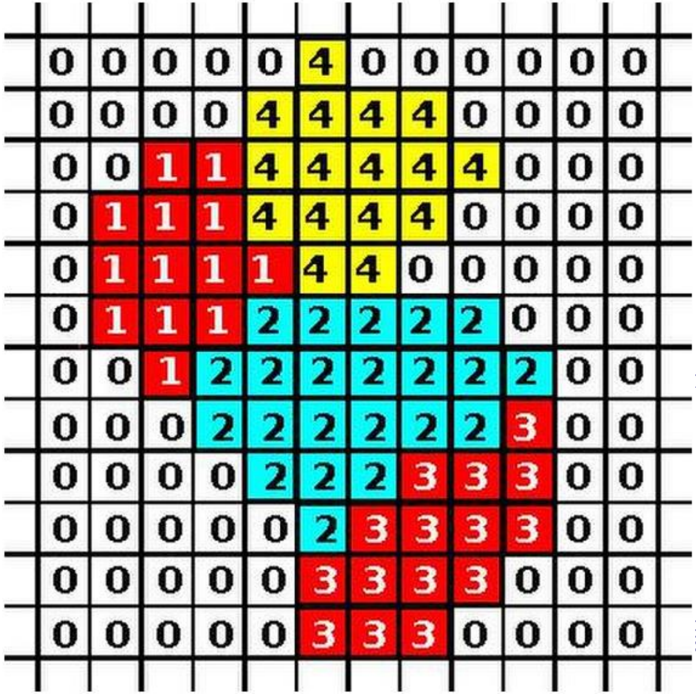
Newman & Girvan 2004; *Newman* 2006; *Wierzbiński*, et al. 2023

Ising-like models

Discovering communities







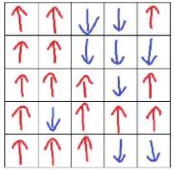
$$\mathscr{H}(\mathbf{h}, \mathbf{J}, \mathbf{s}) = -\sum_i h_i s_i - \frac{1}{2}\sum_{ij} J_{ij} s_i s_j$$

$$\mathscr{H}(\mathbf{h}, \mathbf{J}, \mathbf{s}) = -\sum_i h_i s_i - \frac{1}{2}\sum_{ij} J_{ij} \delta(s_i, s_j)$$

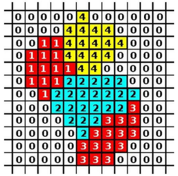
https://stanford.edu/

H-mappings and community *flips*

Discovering communities



$$\mathscr{H}(\mathbf{h},\mathbf{J},\mathbf{s}) = -\sum_i h_i s_i - \frac{1}{2}\sum_{ij} J_{ij} s_i s_j$$

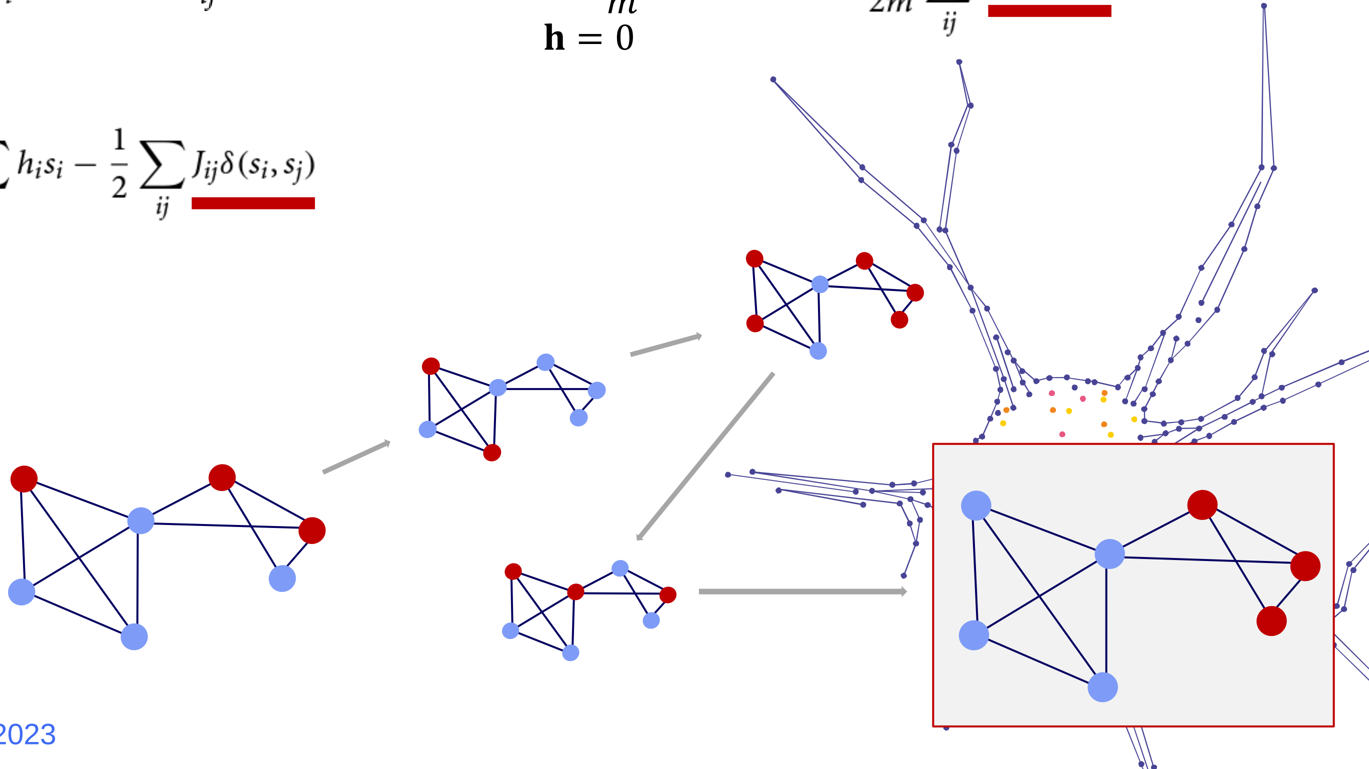


$$\mathscr{H}(\mathbf{h},\mathbf{J},\mathbf{s}) = -\sum_i h_i s_i - \frac{1}{2}\sum_{ij} J_{ij}\delta(s_i, s_j)$$

$$\boldsymbol{J} \doteq -\frac{1}{m}\boldsymbol{B}$$
$$\mathbf{h} = 0$$

$$Q = \frac{1}{2m}\sum_{ij} B_{ij}\delta(c_i, c_j)$$

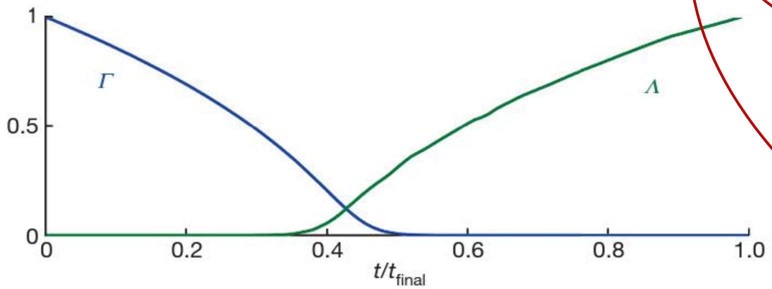
$s_i = +1$ $\quad$ $s_i = -1$

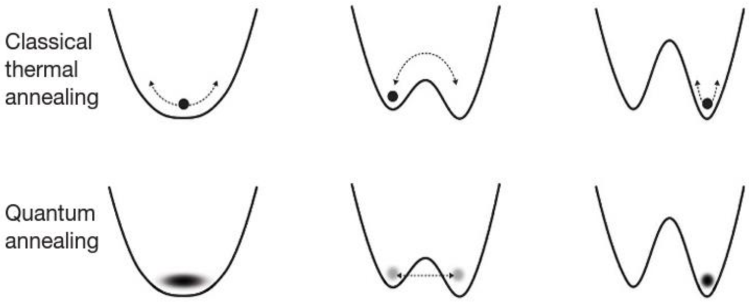


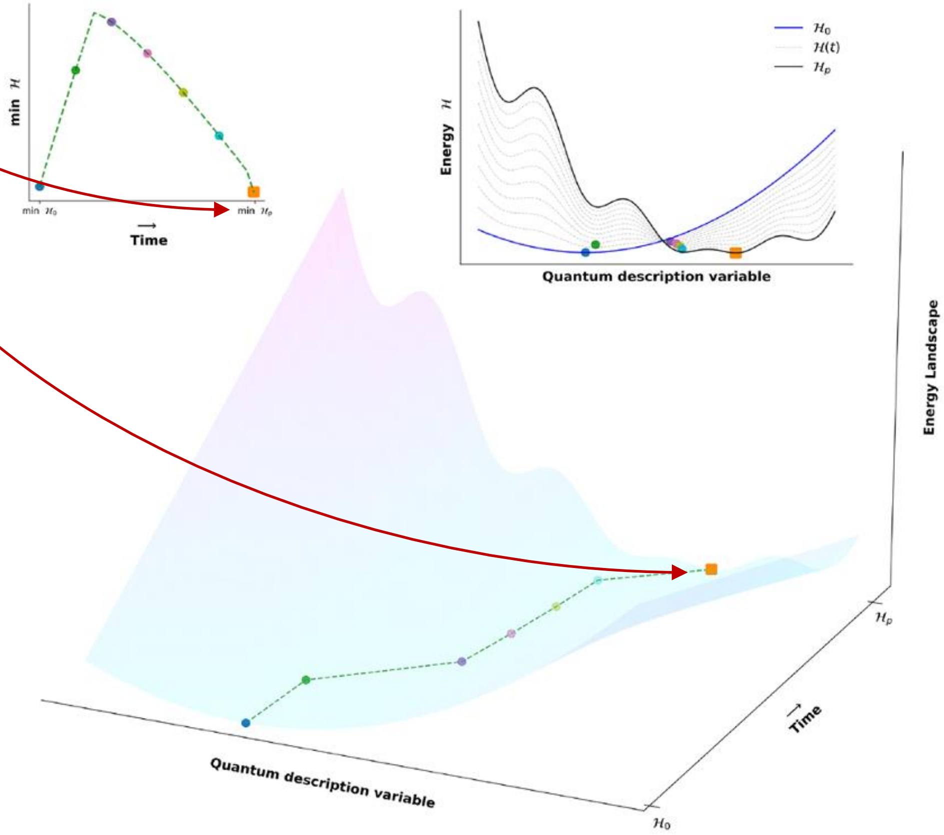
https://stanford.edu/; *Wierzbiński*, et al. 2023

Quantum Adiabatic Optimization

$$\mathscr{H}(t) = \Gamma(t)\mathscr{H}_0 + \Lambda(t)\mathscr{H}_p$$







Johnson, et al. 2011; *Farhi*, et al. 2001; *Rajak*, et al. 2022; *Wierzbiński*, et al. Sci. Rep. 2023

QUBO: BQMs and DQMs

Discovering communities using the *D-wave* API

$$Q = \frac{1}{2m} \sum_{ij} B_{ij} \delta(c_i, c_j)$$

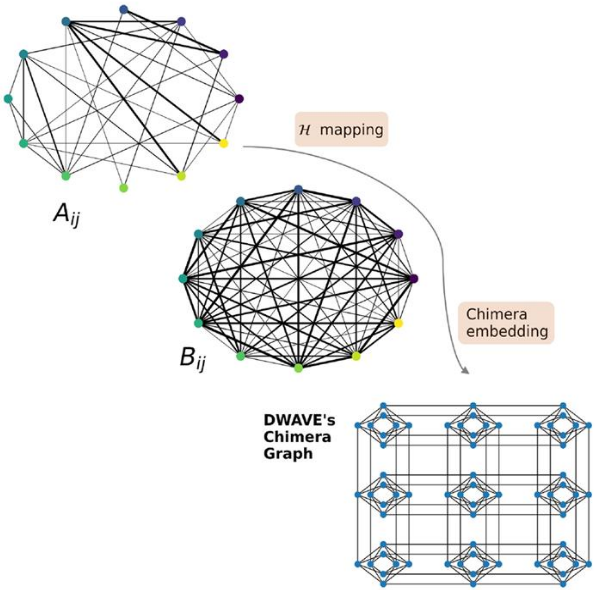
$$\boldsymbol{J} \doteq -\frac{1}{m} \boldsymbol{B}$$

1) $s_i \rightarrow 2x_i - 1$ **K=2** → Binary Quadratic Model (BQM)

2) The Discrete Quadratic Model (DQM) is a bit more tricky

$$\delta(c_i, c_j) \rightarrow \boldsymbol{x} = \begin{pmatrix} 1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 1 \end{pmatrix}$$ is a matrix containing one-hot encodings

$\sum_j x_{ij} = 1 \; \forall j = 1, \ldots, N$ nodes in the network



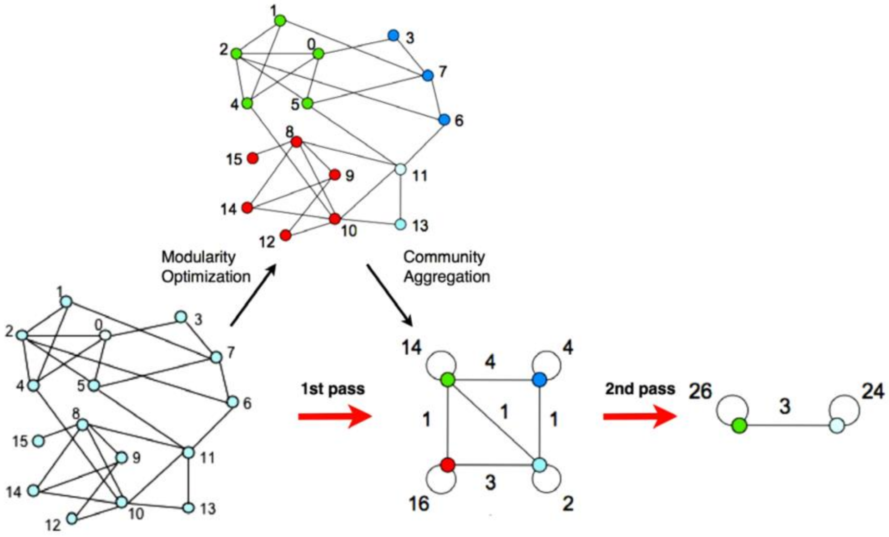

```
import networkx as nx
G = nx.from_numpy_matrix(A)
B = nx.modularity_matrix(G)
from dimod import DiscreteQuadraticModel
from dwave.system import LeapHybridDQMSampler
dqm = DiscreteQuadraticModel()

partitions = range(k)
for i in G.nodes():
      dqm.add_variable(k, label=i)

for i in G.nodes():
  for j in G.nodes():
      if i==j:
          continue
      dqm.set_quadratic(i,j, {(c, c): ((-1)*B[i,j]) for c in partitions})
```

Results

Benchmarking the D-wave Leap Hybrid Solver

1) Louvain Community Detection Algorithm:

$$\Delta Q = \left[\frac{\sum_{\text{in}} + 2k_{i,\text{in}}}{2m} - \left(\frac{\sum_{\text{tot}} + k_i}{2m}\right)^2\right] - \left[\frac{\sum_{\text{in}}}{2m} - \left(\frac{\sum_{\text{tot}}}{2m}\right)^2 - \left(\frac{k_i}{2m}\right)^2\right]$$



Blondel, et al. 2008

Modularity and community structure in networks

M. E. J. Newman*

Finding and evaluating community structure in networks

M. E. J. Newman[1,2] and M. Girvan[2,3]

Community detection in complex networks using extremal optimization

Jordi Duch and Alex Arenas

Fast detection of community structures using graph traversal in social networks

Partha Basuchowdhuri[1] · Satyaki Sikdar[2] · Varsha Nagarajan[1] · Khusbu Mishra[1] · Surabhi Gupta[1] · Subhashis Majumder[1]

Modularity from fluctuations in random graphs and complex networks

Roger Guimerà, Marta Sales-Pardo, and Luís A. Nunes Amaral

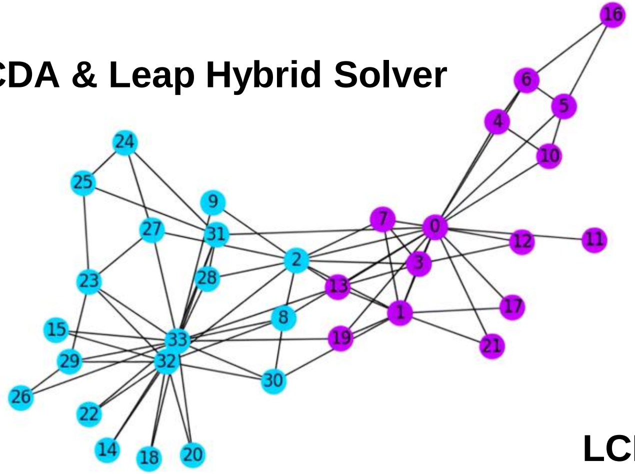
Fast unfolding of communities in large networks

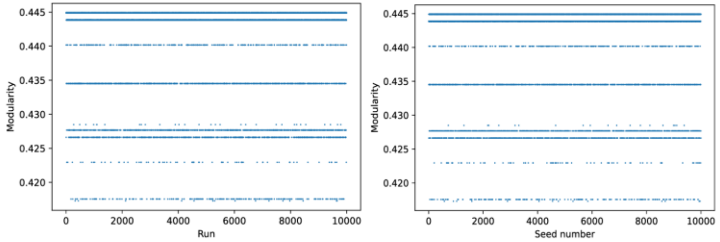
Vincent D Blondel[1], Jean-Loup Guillaume[1,2], Renaud Lambiotte[1,3] and Etienne Lefebvre[1]

Results

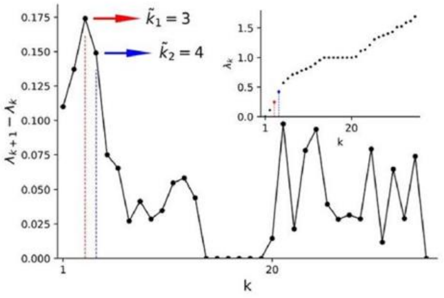
Karate Club

LCDA & Leap Hybrid Solver

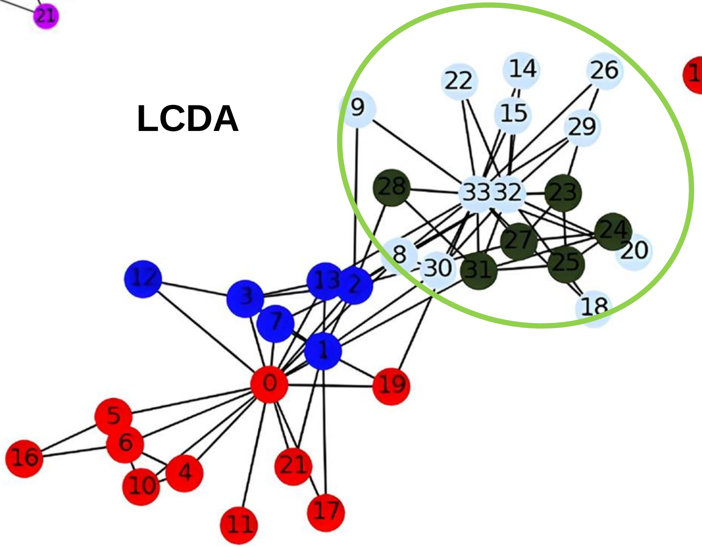




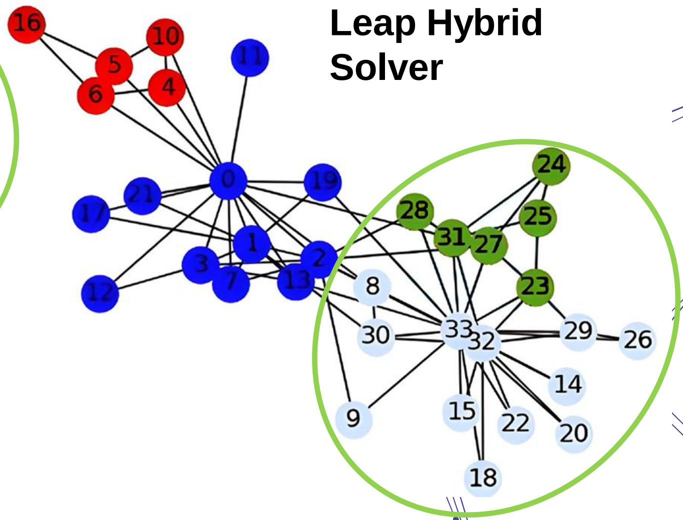
Algorithm	Modularity *Q*	Comp. time (s)	N_{comm}	k_{max}
LCDA	0.440 ± 0.008	**0.003 ± 0.001**	4 (3.9)	4
QA	**0.444 ± 0.000**	3.91 ± 0.12	4 (4)	4



LCDA



Leap Hybrid Solver

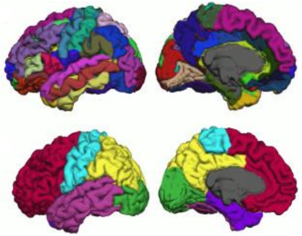


Blondel, et al. 2008

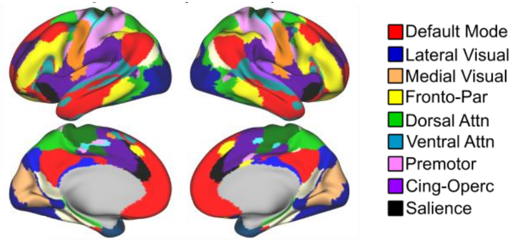
Results

Interpretable communities in bran networks

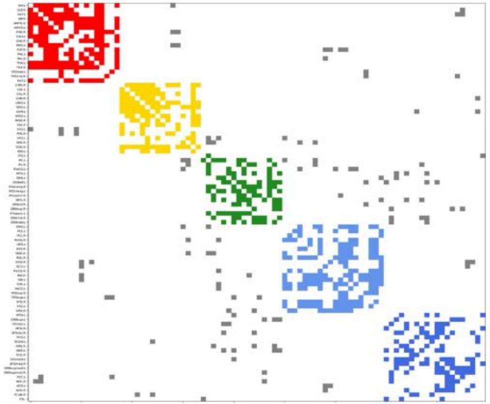
Dosenbach

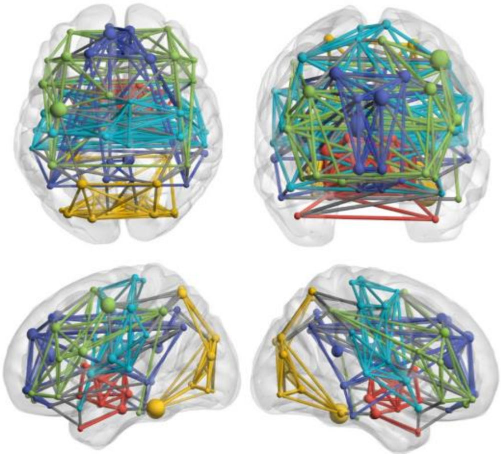


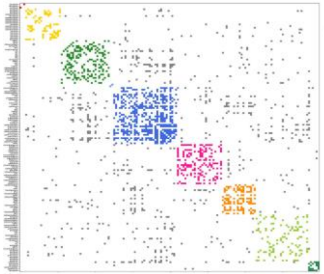
Algorithm	AAL90 ($k_{max} = 11$)			Dosenbach ($k_{max} = 27$)		
	Modularity Q	Comp. Time (s)	N_{comm}	Modularity Q	Comp. Time (s)	N_{comm}
LCDA	0.644 ± 0.003	**0.002 ± 0.001**	6 (5.7)	0.404 ± 0.006	**0.005 ± 0.001**	13 (12.96)
QA	**0.648 ± 0.000**	5.3 ± 0.1	5 (5)	**0.416 ± 0.000**	5.4 ± 0.1	9 (9)

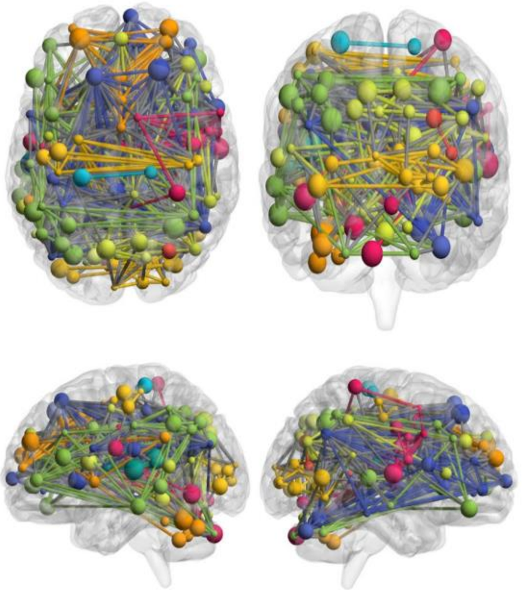


Automated Anatomically Labelled (AAL90)









Conclusions

1) Key points

- Rigorous description of spin-like variables and models to find modular organizations

- Modularity maximization is an NP-hard problem potentially solvable using Quantum Annealing (*Farhi,* et al. 2001)

- The *quantum* approach is capable of rendering efficient community structures: **highly modular**

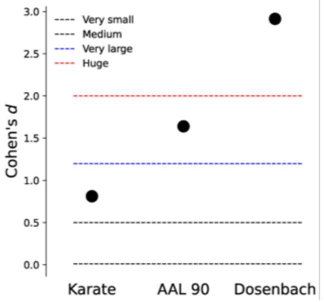
- "**All at once**" method, as opposed to previous attempts (*Negre,* et al. 2020)

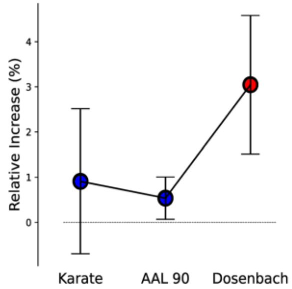
- Solutions seem to be more stable than classical *heuristics*

2) Key limitations

- Computational time ➔ Difficult to determine the origin of this!

- *D-wave* solvers are blacker than black itself! Leap Hybrid Solver allocates the problems by parts to the quantum processing unit





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Future directions

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- How do these type of methods scale with population studies? Is the computational time more stable than classical alternatives?

- Can we get rid of the *classical* part of the workflow? Can we remove the *hybrid* prefix?

- Alternatively, what other solvers prove to be useful for this kind of problems? (CQM, Advantage, …)

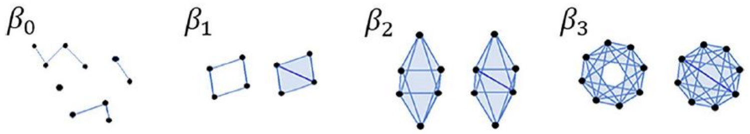
- Other optimization approaches ➔ Hopfield networks (*Rebentrost*, et al. 2018; *Miller & Mukhopadhyay* 2021)

- Other NP-Hard open problems in Network (neuro)science (*Lucas*, et al. 2010) ➔ *The clique problem*

frontiers in PHYSICS

Ising formulations of many NP problems

*Andrew Lucas**



Acknowledgements

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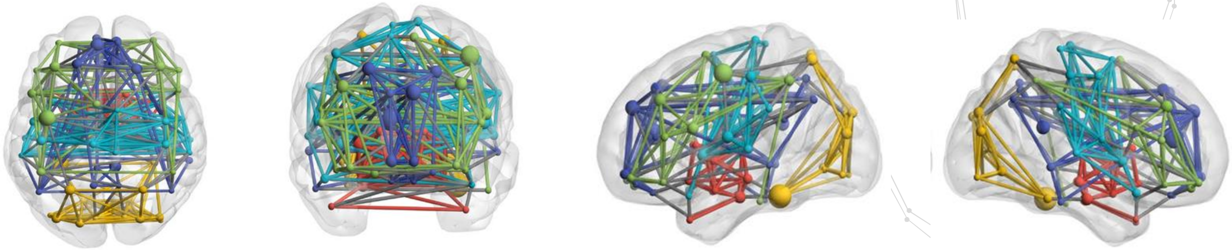
Community detection in brain connectomes with hybrid quantum computing

Marcin Wierzbiński[1,2,3], Joan Falcó-Roget[2,3] & Alessandro Crimi[2]✉



Wierzbiński, M., Falcó-Roget, J. & Crimi, A. Community detection in brain connectomes with hybrid quantum computing. *Sci Rep* **13**, 3446 (2023). https://doi.org/10.1038/s41598-023-30579-y