Title: Solving 2D quantum matter with neural quantum states

Speakers:

Collection: Machine Learning for Quantum Many-Body Systems

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Abstract: Neural quantum states (NQSs) have emerged as a novel promising numerical method to solve the quantum many-body problem. However, it has remained a central challenge to train modern large-scale deep network architectures to desired quantum state accuracy, which would be vital in utilizing the full power of NQSs and making them competitive or superior to conventional numerical approaches. Here, we propose a minimum-step stochastic reconfiguration (MinSR) method that reduces the optimization complexity by orders of magnitude while keeping similar accuracy as compared to conventional stochastic reconfiguration. MinSR allows for accurate training on unprecedentedly deep NQS with up to 64 layers and more than 105 parameters in the spin-1/2 Heisenberg J1-J2 models on the square lattice. We find that this approach yields better variational energies as compared to existing numerical results and we further observe that the accuracy of our ground state calculations approaches different levels of machine precision on modern GPU and TPU hardware. The MinSR method opens up the potential to make NQS superior as compared to conventional computational methods with the capability to address yet inaccessible regimes for two-dimensional quantum matter in the future.

SOLVING 2D QUANTUM MATTER WITH NEURAL QUANTUM STATES

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Workshop "Machine Learning for Quantum Many-Body Physics" 06/15/2023

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European Research Council
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THE QUANTUM MANY-BODY PROBLEM

GROUND STATES AND DYNAMICS

HAMILTONIAN

EIGENSTATES
ground state

$$H|E\rangle = E|E\rangle$$

DYNAMICS

$$i\frac{d}{dt}|\psi(t)\rangle = H|\psi(t)\rangle$$

A KEY CHALLENGE

INTERACTING QUANTUM MATTER IN 2D

SOLVING THE QUANTUM-MANY PROBLEM IS DIFFICULT

Complexity is a matter of the method

EXACT DIAGONALIZATION	TENSOR NETWORKS	QUANTUM MONTE CARLO
Curse of dimensionality	Entanglement Contraction complexity	Sign problem

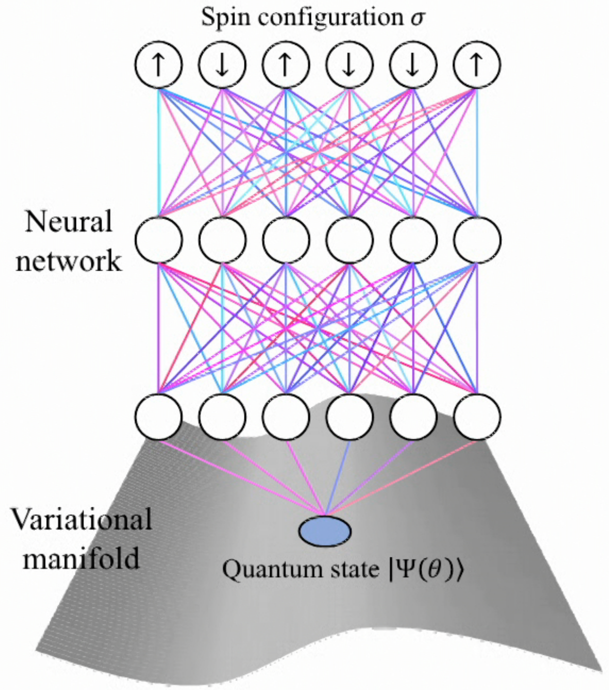
NEURAL QUANTUM STATE (NQS)

NOVEL CLASS OF VARIATIONAL WAVE FUNCTIONS

QUANTUM STATES IN COMPUTATIONAL BASIS

$$|\psi\rangle = \sum_s \psi_s |s\rangle$$

encode into an artificial neural network (ANN)



Carleo & Troyer, Science '17

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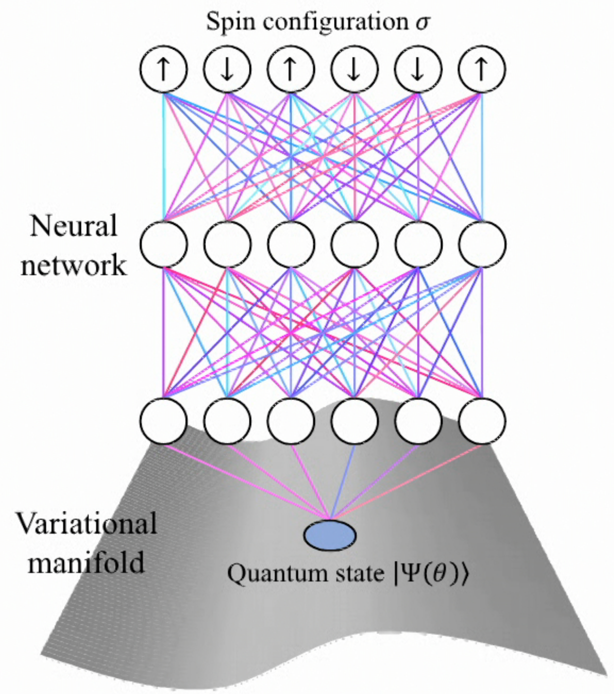

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UNIVERSAL APPROXIMATION THEOREM

Numerically exact approach

Convergence parameter: size of ANN

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GROUND STATES OF COMPLEX 2D QUANTUM MATTER

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GROUND STATES

STOCHASTIC RECONFIGURATION (SR)

NQS IS A VARIATIONAL WAVE FUNCTION

$$|\psi(\theta)\rangle = \sum_s \psi_s(\theta)|s\rangle$$

GROUND STATE: Minimize variational energy

$$\mathcal{E}(\theta) = \frac{\langle\psi(\theta)|H|\psi(\theta)\rangle}{\langle\psi(\theta)|\psi(\theta)\rangle}$$

SR: Imaginary time evolution (from random initial condition)

$$S\dot{\theta} = F \quad \Rightarrow \dot{\theta} = S^{-1}F$$

ONE KEY CHALLENGE

MATRIX INVERSION COMPLEXITY

$$S\dot{\theta} = F \qquad \Rightarrow \dot{\theta} = S^{-1}F$$

CHALLENGE: $S \in \mathbb{C}^{N_p \times N_p}$ $\quad N_p$: number of variational parameters

Computational complexity for inversion: $\mathcal{O}(N_p^3)$

LIMITS CRITICALLY THE REACHABLE ANN SIZES

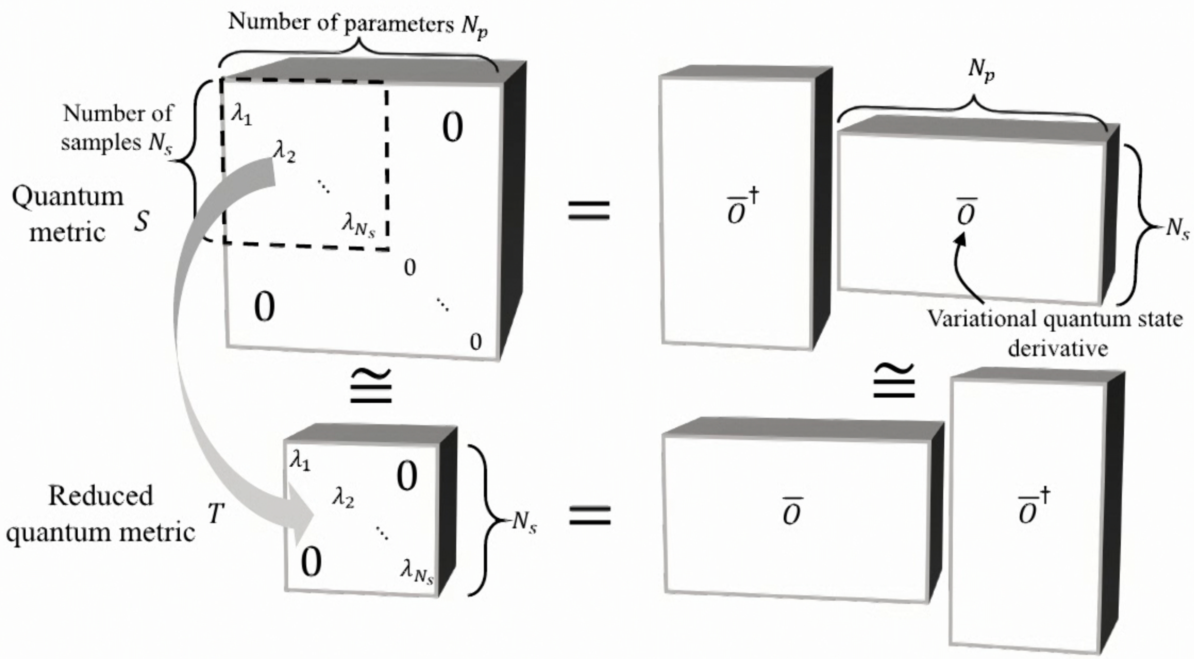
SOLUTION: Minimum-step stochastic Reconfiguration

Chen & **MH** arXiv:2302.01941

Reducing the computational complexity: $\mathcal{O}(N_p)$

A NEW OPTIMIZER: MINSR

NEURAL TANGENT KERNEL

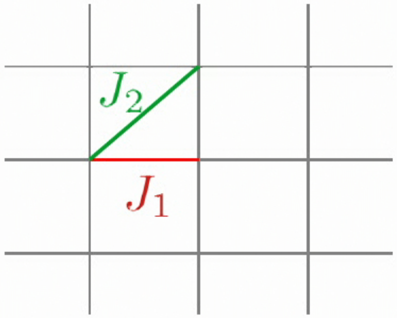


$$\delta\theta = S^{-1}\overline{O}^\dagger\overline{\epsilon} \quad \text{with}\, S = \overline{O}^\dagger\overline{O} \quad \rightarrow \quad \delta\theta = \overline{O}^\dagger T^{-1}\overline{\epsilon} \quad \text{with}\, T = \overline{O}\,\overline{O}^\dagger$$

ANTIFERROMAGNETIC HEISENBERG MODEL

SQUARE LATTICE

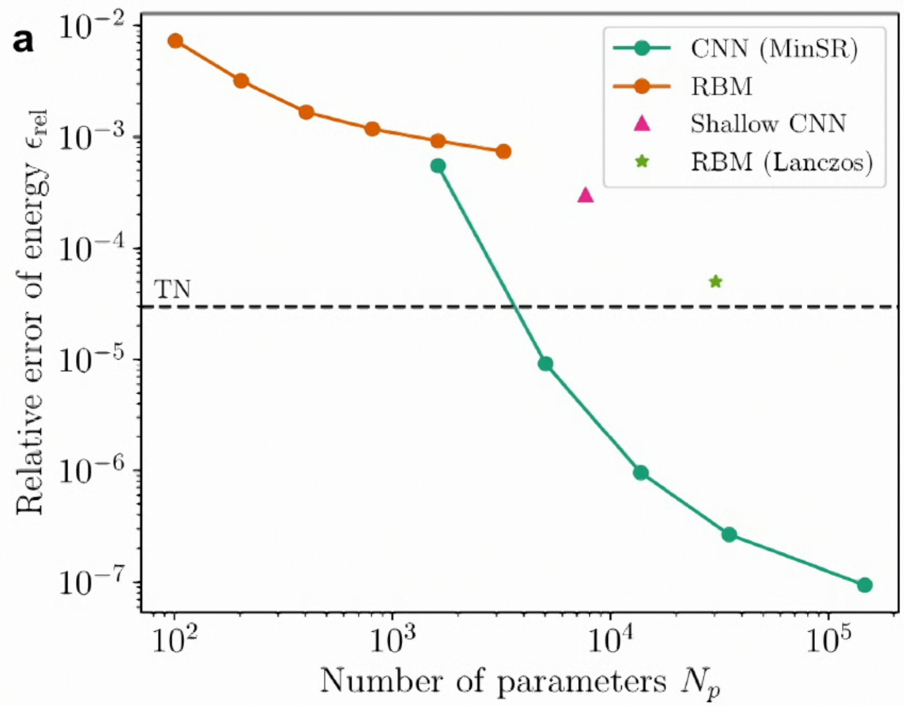
$$\mathcal{H} = J_1 \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$



HEISENBERG MODEL

APPROACHING MACHINE PRECISION

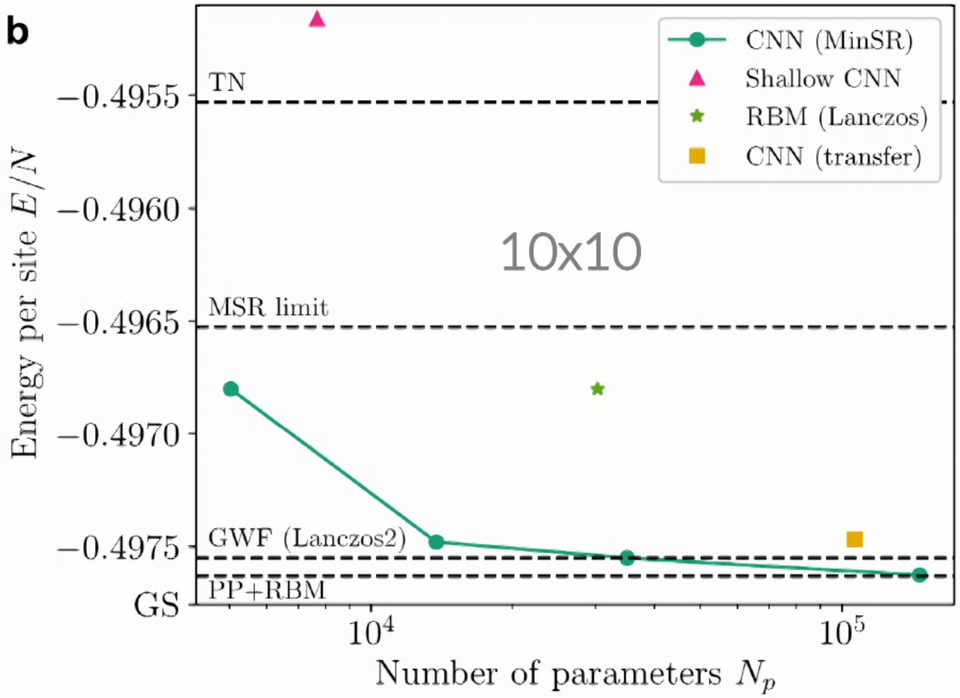
10x10



Chen & MH arXiv:2302.01941

J1-J2 MODEL

FRUSTRATED POINT J2/J1=1/2



16x16

Wave function	Reference	E/N
PP+RBM	[7]	−0.496213(3)
GCNN	[9]	−0.496407(7)
CNN(transfer)	[29]	−0.49659
CNN(MinSR)	This work	−0.496683(2)

Chen & MH arXiv:2302.01941

DYNAMICS OF COMPLEX 2D QUANTUM MATTER

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FZ Jülich → Regensburg

QUANTUM DYNAMICS

TIME-DEPENDENT VARIATIONAL PRINCIPLE

$$i\frac{d}{dt}|\psi(t)\rangle = H|\psi(t)\rangle$$

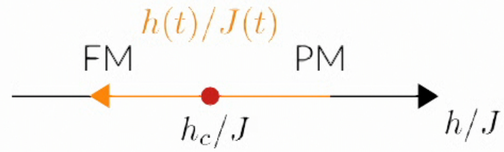
TIME-DEPENDENT VARIATIONAL PRINCIPLE

$$S\dot{\theta} = iF$$

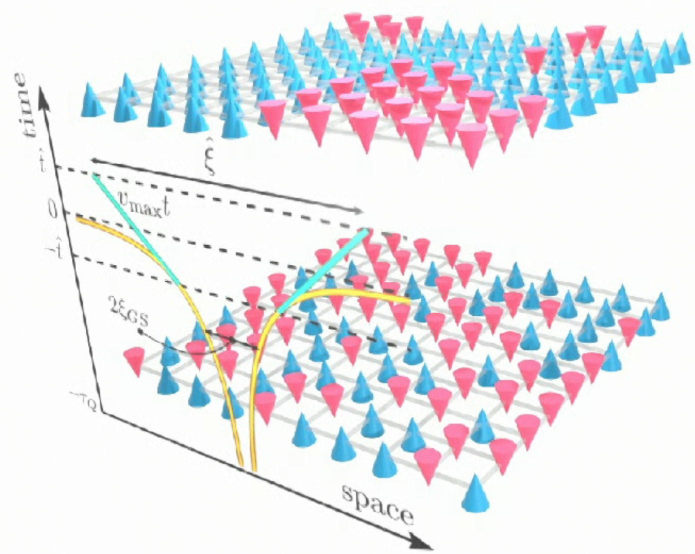
QUANTUM KIBBLE-ZUREK MECHANISM

DYNAMICAL UNIVERSALITY FOR INTERACTING 2D QUANTUM MATTER

$$H = -J \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z - h \sum_j \sigma_j^x$$



$$\hat{\xi} \propto \tau_Q^{\nu/(1+z\nu)}$$



Well-established in 1D
What is special about 2D?

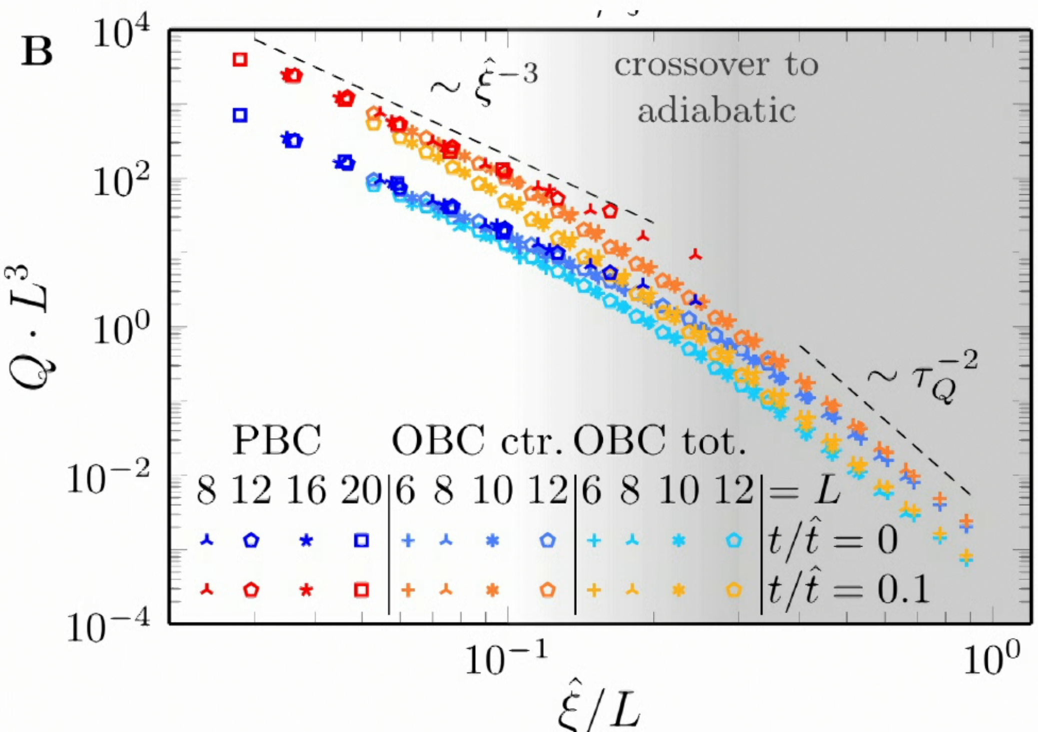
Conformal field theories fundamentally different!

M. Schmitt, **MH**, et al. Science Advances '22

UNIVERSAL DEFECT PRODUCTION

2D QUANTUM ISING MODEL

Excess energy



M. Schmitt, MH, et al. Science Advances '22

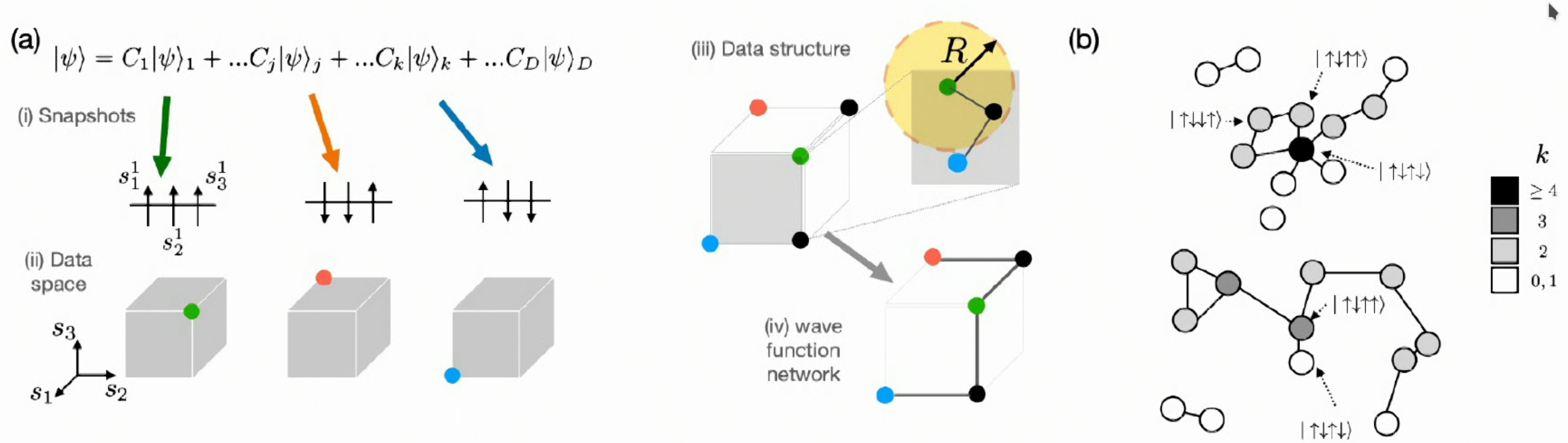
QUANTUM WAVE FUNCTION NETWORKS

CONSTRUCTING NETWORKS FROM SNAPSHOT MEASUREMENTS

SNAPSHOTS AS DATA SETS

IMPOSING STRUCTURE

RESULTING NETWORKS

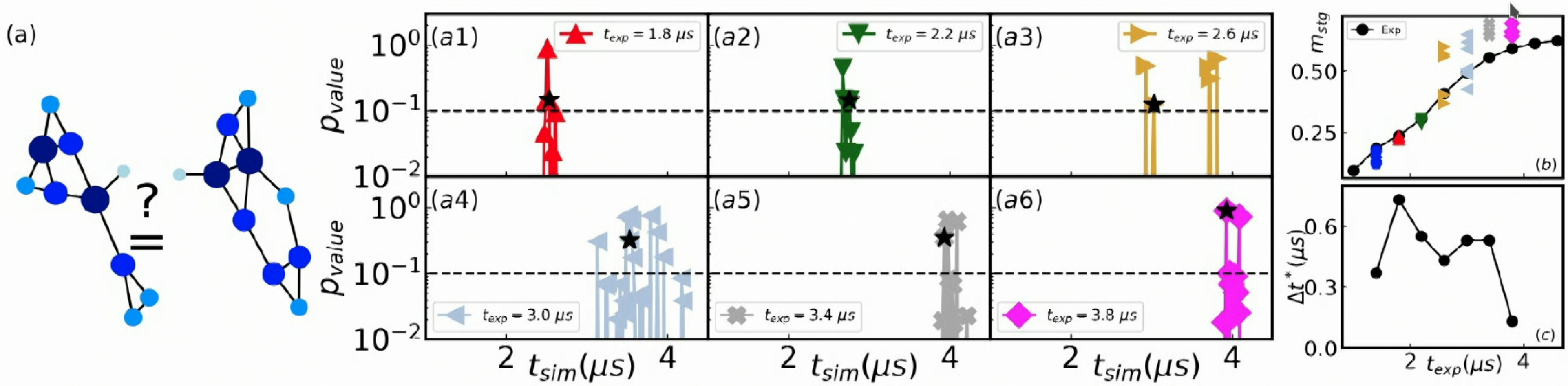


T. Mendes-Santos, MH, et al. arXiv:2301.13216

CROSS CERTIFICATION

COMPARING NETWORK STRUCTURES

EPPS-SINGLETON TEST



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