Data-driven discovery of relevant information in many-body problems

Roberto Verdel Aranda
ICTP, Trieste

arXiv:2307.10040
arXiv:2308.13636

"Many-Body quantum physics with machine learning"
ECT*, Trento
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The Abdus Salam International Centre for Theoretical Physics

ECT*
EUROPEAN CENTRE FOR THEORETICAL STUDIES IN NUCLEAR PHYSICS AND RELATED AREAS

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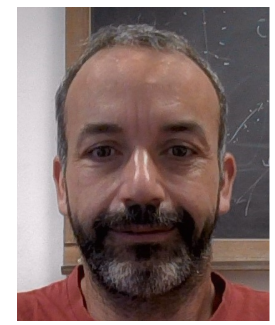

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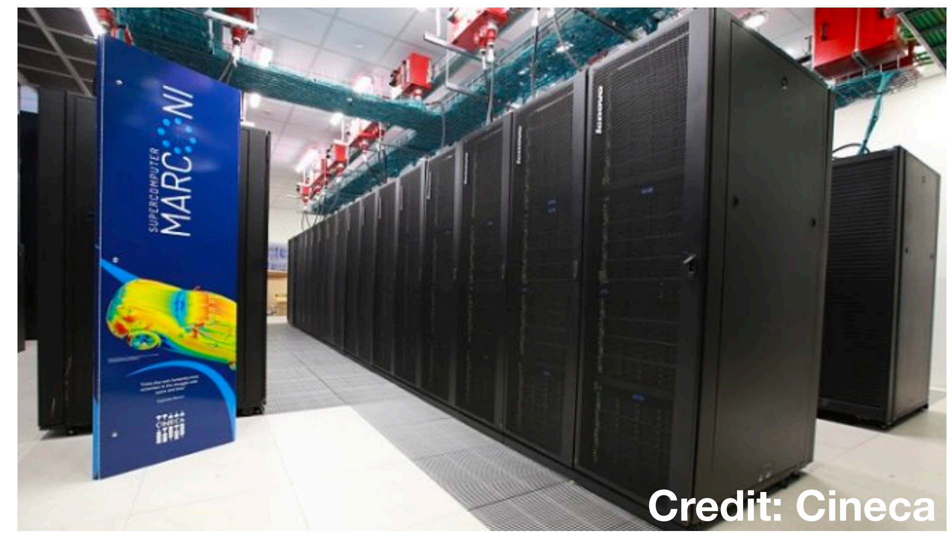
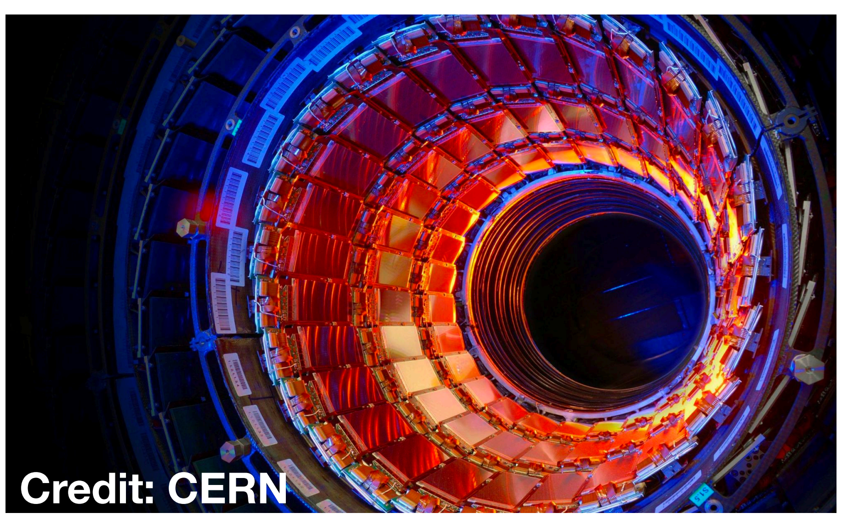
Motivation I: Physics in the age of big data

- Astrophysical observations

- Large-scale classical simulations



- Particle physics experiments



- Quantum simulation

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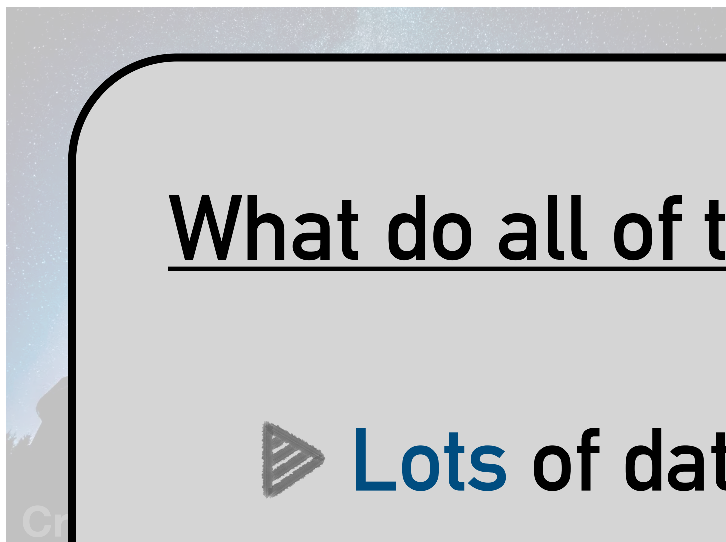

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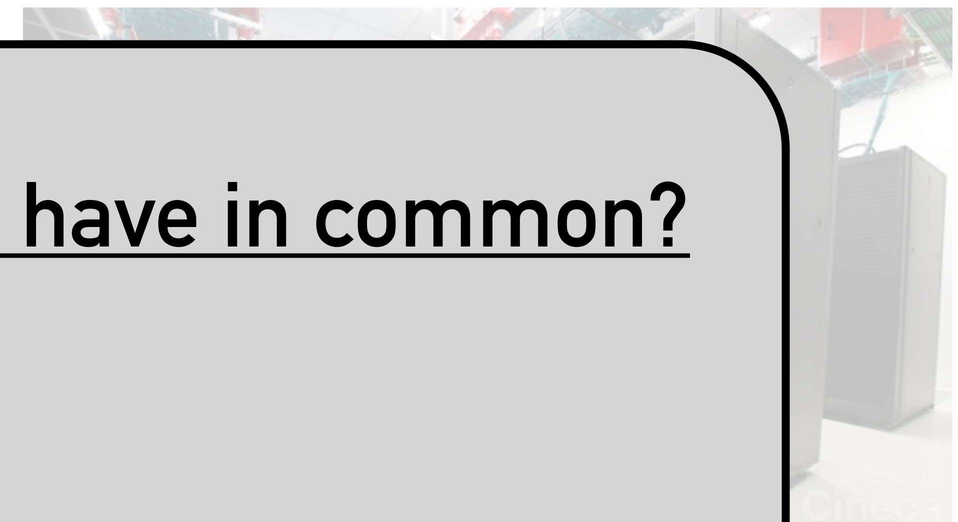
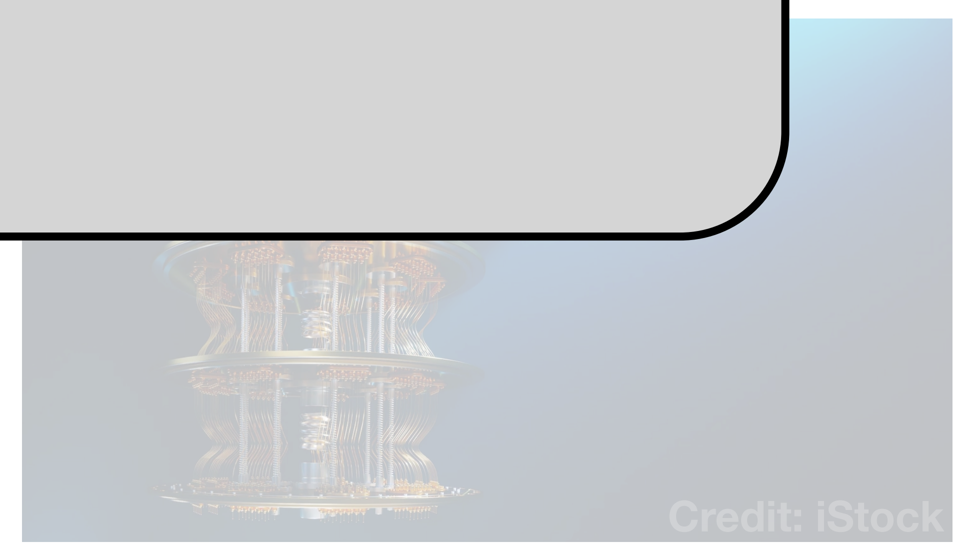


- Particle



<u>What do all of these fields have in common?</u>

- Lots of data available
- Data mining/ML methods can enable/ facilitate discovery

Motivation II: Quantum technology era

Present-day synthetic quantum devices offer an unparalleled way to probe correlated quantum matter

- Coherent dynamics with control at the individual quantum level
- Capable to produce "wave function snapshots"

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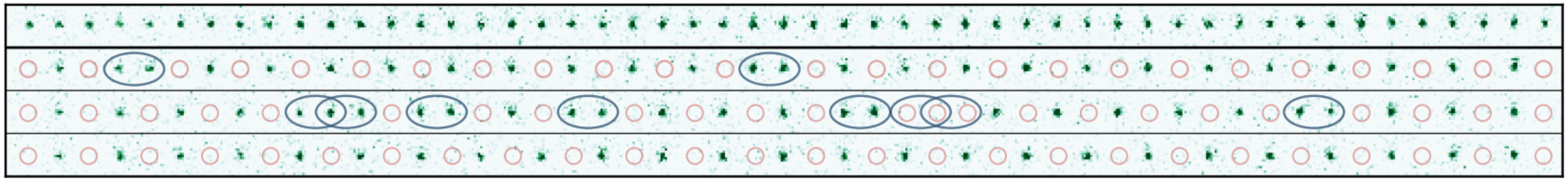

Bernien et al., Nature '17

$$\vec{X}_i = (0,1,0,1,0,1,\ldots) \qquad \mathbf{M} = \{\vec{X}_1, \vec{X}_2, \ldots, \vec{X}_{N_r}\}$$

Motivation II: Quantum technology era

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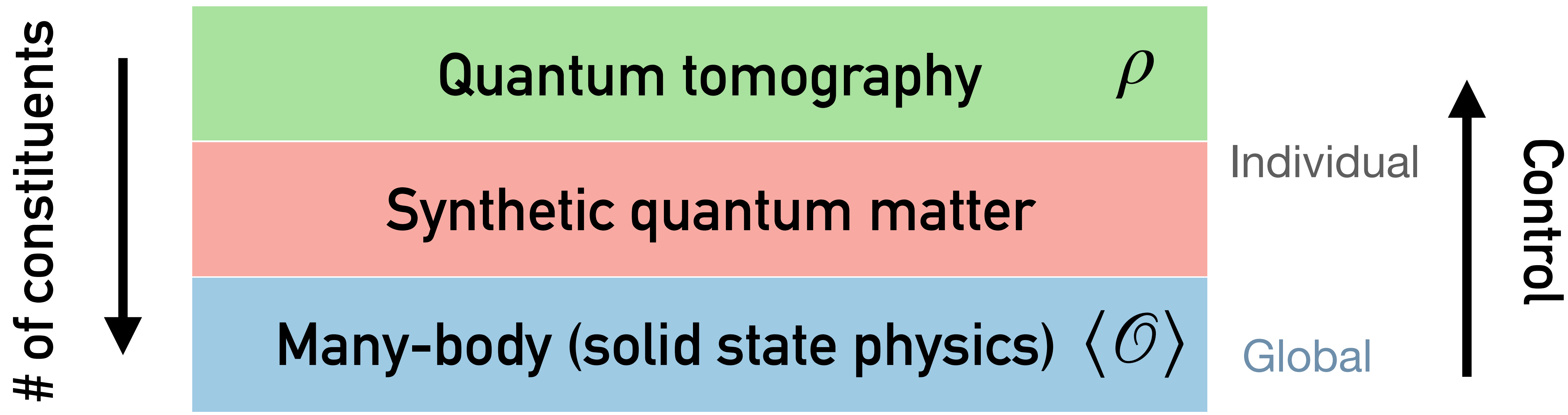


Motivation II: Quantum technology era

Present-day synthetic quantum devices offer an unparalleled way to probe correlated quantum matter

How can we deal with the full information content of many-body snapshots provided by synthetic quantum systems?

# of constituents

Synthetic quantum matter

Many-body theory $\langle \mathcal{O} \rangle$

Control

A couple of remarks

- Output of quantum simulations are classical objects. Hence data-wise equivalent to output of classical simulations (the techniques I will discuss today can also be applied to classical simulations).
- We work with limited sampling: $N_s \ll 2^N$.
- Complementary to other techniques such as classical shadows, randomised measurements, etc.

How do we extract relevant information from many-body snapshots?

"Traditional" approaches (stat mech / effective field theory):
compute few-point correlators, for instance:

$$C_{ij}^{(2)} = \langle x_i x_j \rangle - \langle x_i \rangle \langle x_j \rangle$$

Allows us to characterize classical/quantum phase transitions, determine "proper vertices" of the quantum effective action, etc.

However, it disregards part of the information content of many-body snapshots	In data science jargon: an "uncontrolled" dimensional reduction

Why we would like to go beyond?

- Unbiased identification the relevant degrees of freedom at play in strongly interacting theories

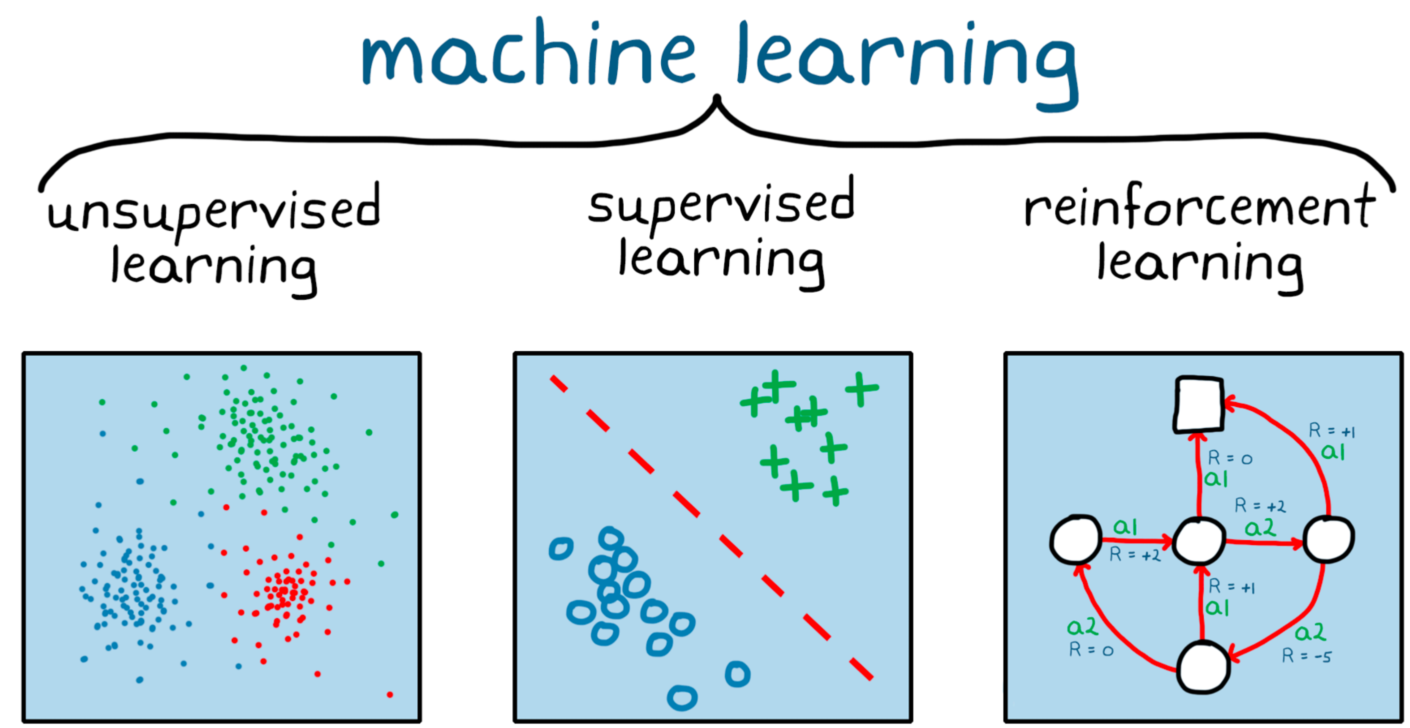
- Understanding the working of quantum computers (e.g. choosing best suited measurement basis, cross-platform verification, noise tomography, etc.)

- Quantifying the complexity of wave functions

- Detect and characterise systems with non-local correlations (topological phases of matter)

Data-driven strategy

Use non-parametric unsupervised approaches to discover and extract relevant information in many-body physics problems by leveraging all available information

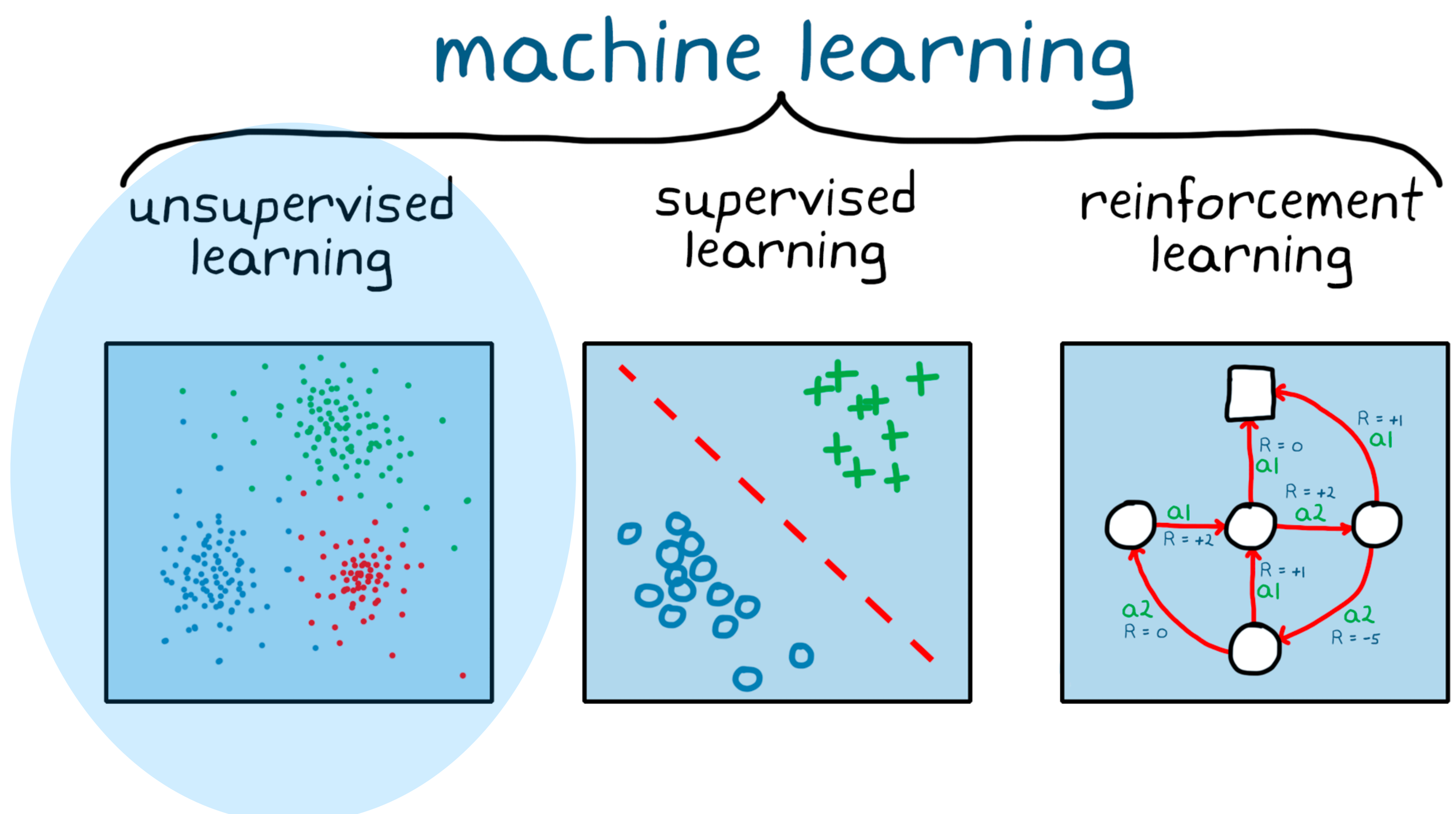


https://www.mathworks.com/discovery/reinforcement-learning.html

Data-driven strategy

Use non-parametric unsupervised approaches to discover and extract relevant information in many-body physics problems by leveraging all available information

Think of methods related to dimensional reduction, feature selection, etc.



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Technical outline

- Learning critical behaviour in Ising partition functions
  - Intrinsic dimension
  - PCA-based entropy

arXiv:2308.13636

- Relevant information discovery in quantum simulators
  - Ranking operators via PCA entropy and information imbalance*
  - Complexity of universal dynamics far from equilibrium

arXiv:2307.10040

Similar approaches

Stat mech / lattice field theory:

Hu et al. PRE '17
Wetzel PRE '17
Wang & Zhai, PRB '17
Ch'ng et al., PRE '18
Mendes-Santos et al., PRX '21
Sale et al., PRE '22; PRD '23
Sehayek & Melko, PRB '22
Spitz, et al., PRD '23
Vitale et al., arXiv '23

Quantum many-body:

Rodriguez-Nieva & Scheurer, Nat Phys '19
Lidiak & Gong, PRL '20
Mendes-Santos et al., PRX Quantum '21
Bohrdt et al., PRL '21
Spitz, et al., SciPost Phys '21
Tirelli & Costa, PRB '21
Schmitt & Lenarčič, PRB '22
Miles et al., PRR '23
Mendes-Santos et al., arXiv '23

… and many more!

Learning critical behaviour in Ising partition functions

Rajat Panda

arXiv:2308.13636; see also arXiv 2308.13604

Intrinsic dimension

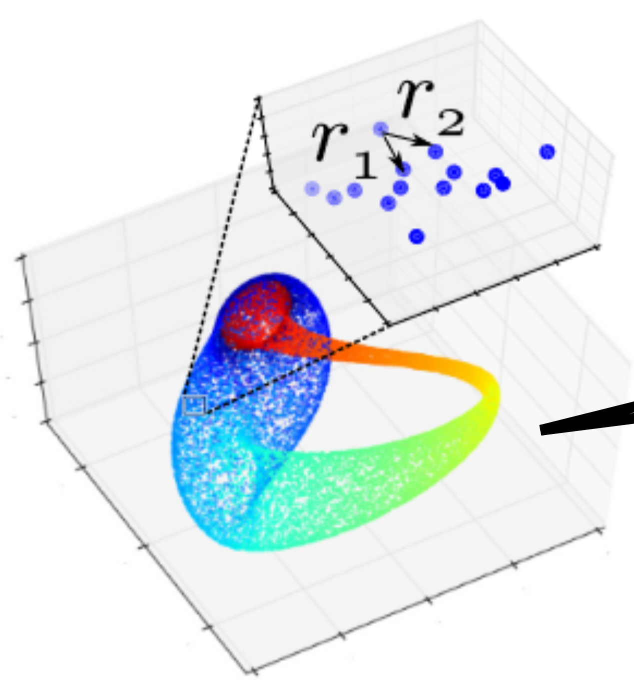
- Basic tool in data mining with multiple applications in chemical and bimolecular science and image analysis

Glielmo et al., Chem. Rev. ‘21

- Quantifies the minimum number of variables needed to describe the data

- Serves as a proxy of the Kolmogorov complexity

$D = 3$



$I_d = 2$

Each point is, for example, a spin configuration

Mendes-Santos et al., PRX ‘21

Intrinsic dimension: TWO-NN

Facco et al., Sci. Rep. '17

Uses statistics of distances between nearest-neighbor (NN) points

Needs a metric (e.g. for spin systems: Hamming distance)

$$d(i,j) := \sum_r | \vec{S}_r^i - \vec{S}_r^j |$$

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Facco et al., Sci. Rep. '17

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Example: 3-site system

$$\vec{S}^1 = (0,1,1)$$

$$\vec{S}^2 = (1,1,1)$$

$$\vec{S}^3 = (1,0,1)$$

$$\vec{S}^4 = (0,0,0)$$

$$d(\vec{S}^1, \vec{S}^2) = |0-1| + |1-1| + |1-1| = 1$$

$$d(\vec{S}^1, \vec{S}^3) = 2$$

$$\ldots$$

Intrinsic dimension: TWO-NN

Facco et al., Sci. Rep. '17

Uses statistics of distances between nearest-neighbor (NN) points

Needs a metric (e.g. for spin systems: Hamming distance)

Main assumption: NN points are drawn uniformly from I_d-dim hyperspheres

For each point, compute:

$$\mu = \frac{r_2}{r_1}$$

Distribution function of μ:

$$f(\mu) = \frac{I_d}{\mu^{I_d+1}}$$

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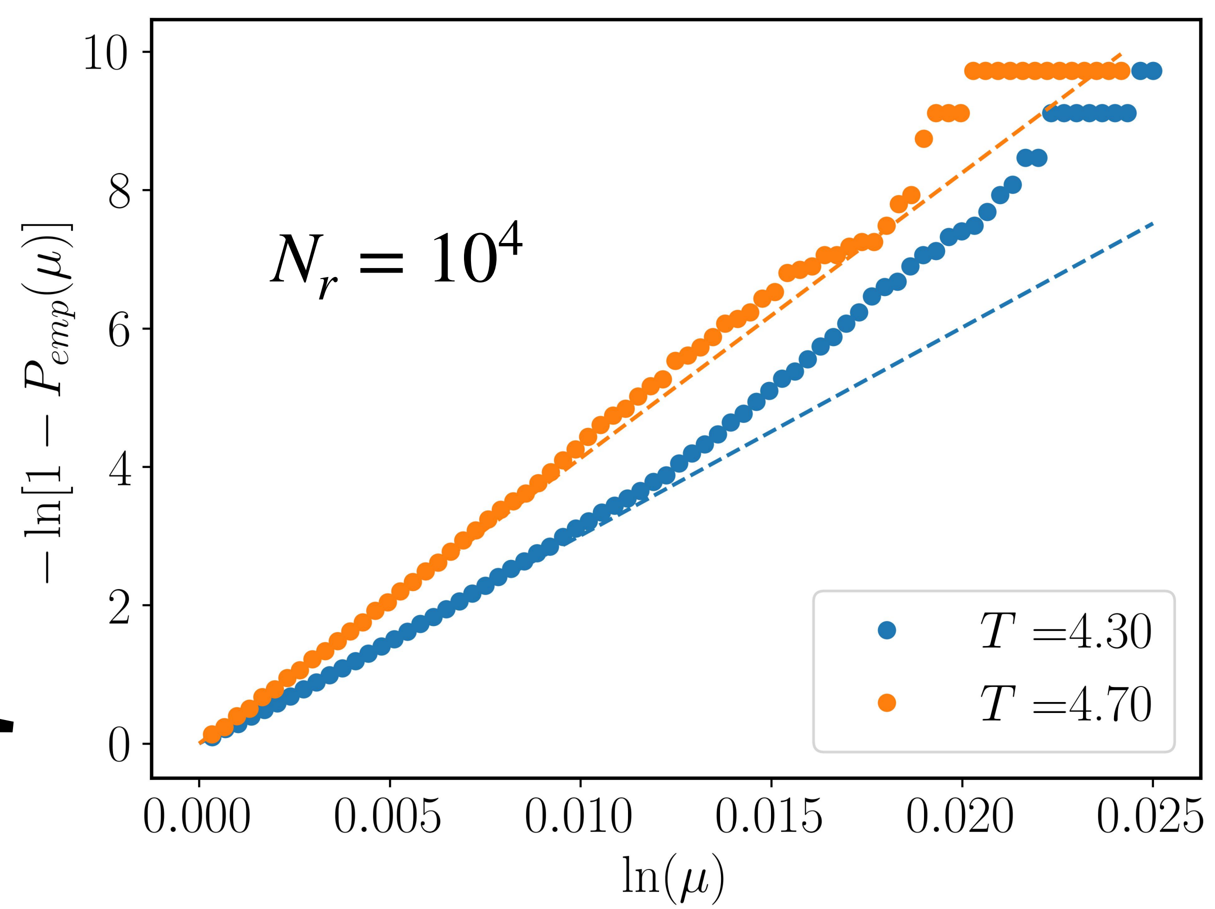
Linear fit using cumulative dist. function



Intrinsic dimension: toy example

Toy example: 3-site XY model

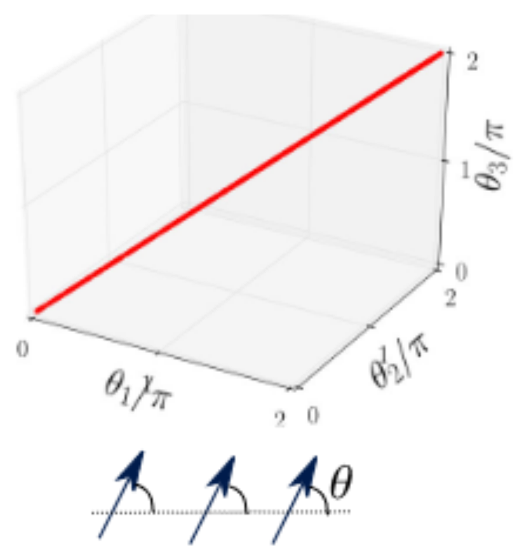
Mendes-Santos et al., PRX '21

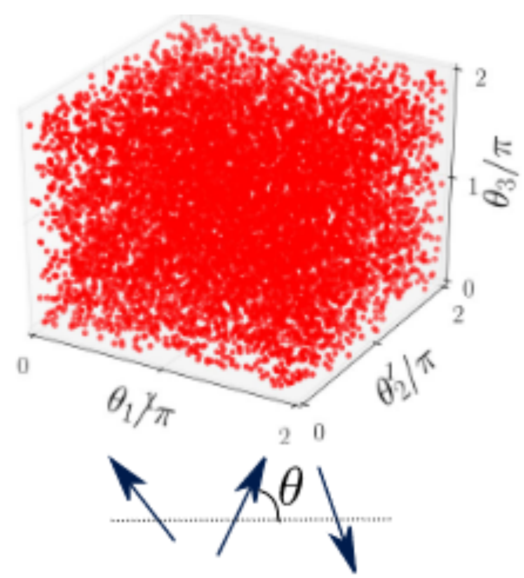
Hamiltonian: $$H = -\sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j)$$

Configurations (data points): $(\theta_1, \theta_2, \theta_3)$

Low temperature

$I_d = 1$





High temperature

$I_d = D = 3$

What about close to a transition point?

Intrinsic dimension: 2D Ising

<u>2D classical Ising model</u>

$$E = -J \sum_{\langle i,j \rangle} S_i S_j$$

Square lattice

Divergent correlation length: do data structures are more complex?

Second-order (conformal) phase transition

$$T_c = \frac{2}{\ln(1+\sqrt{2})} \approx 2.269$$

$$\nu = 1$$

Mendes-Santos et al., PRX '21

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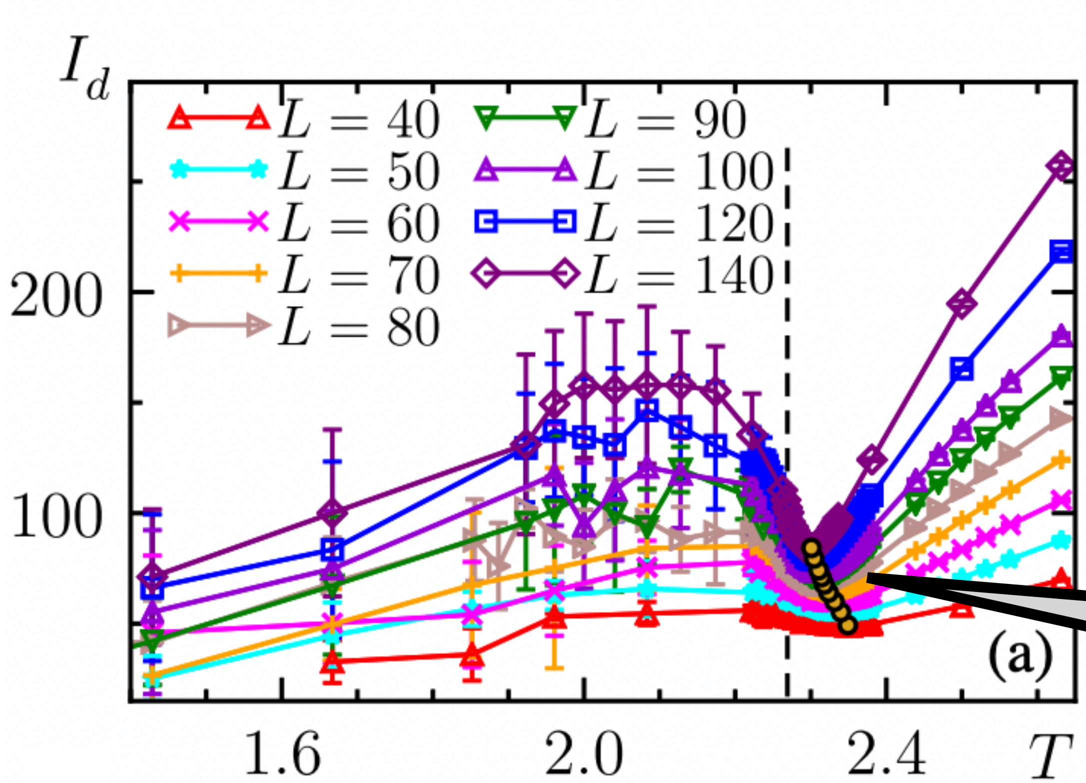

Manifold simplifies at the transition!

Intuition: universality

Mendes-Santos et al., PRX '21

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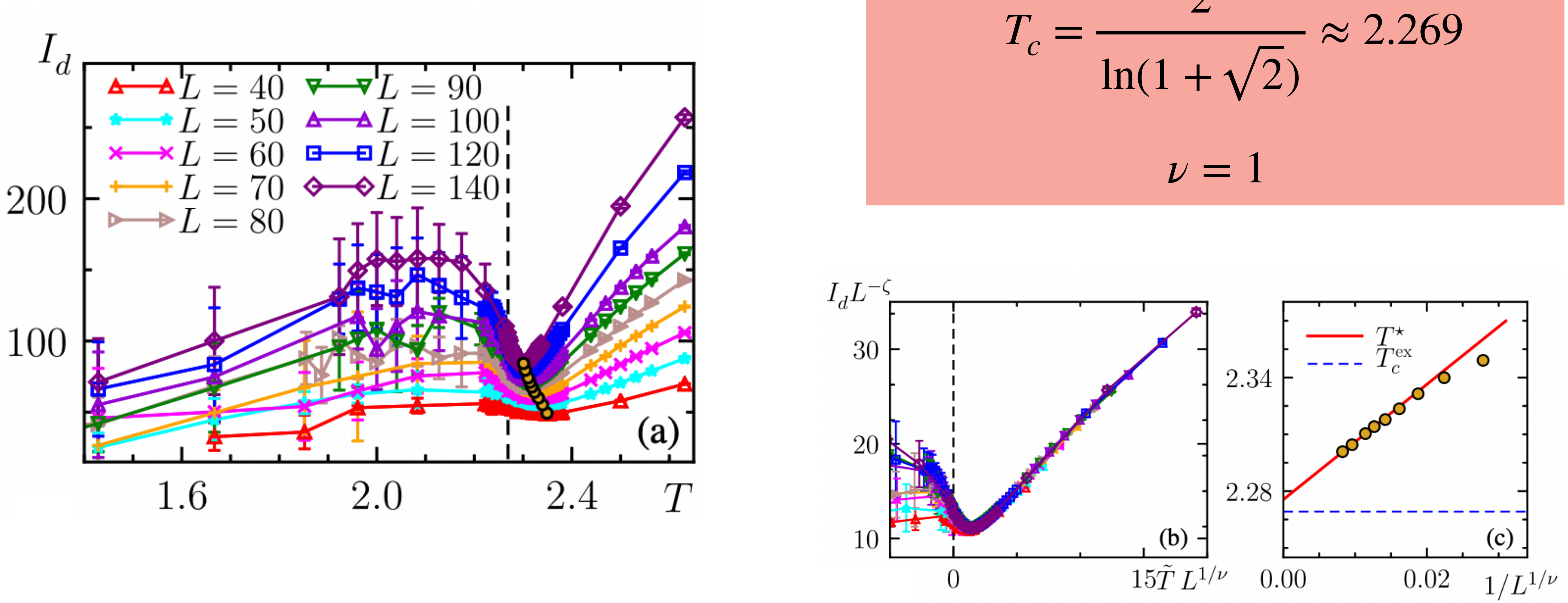
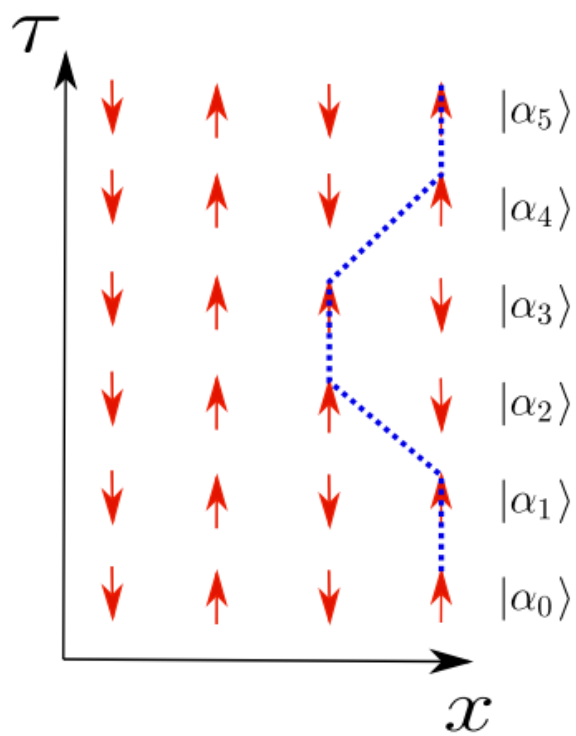
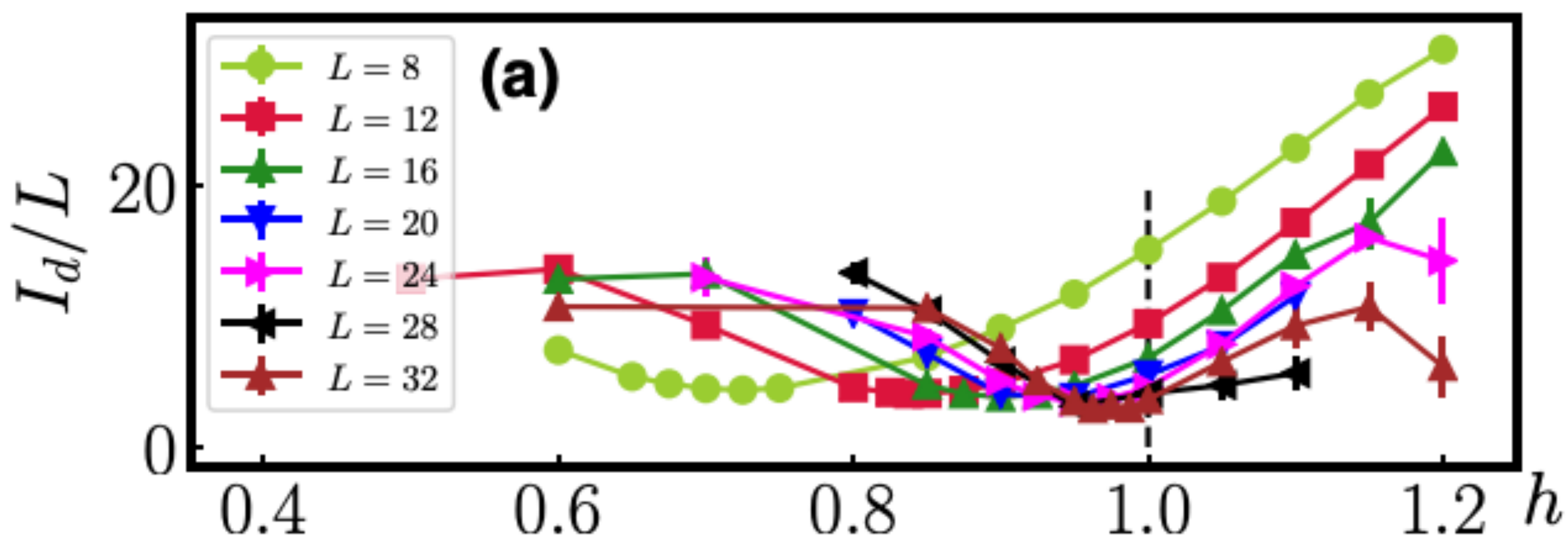


Mendes-Santos et al., PRX '21

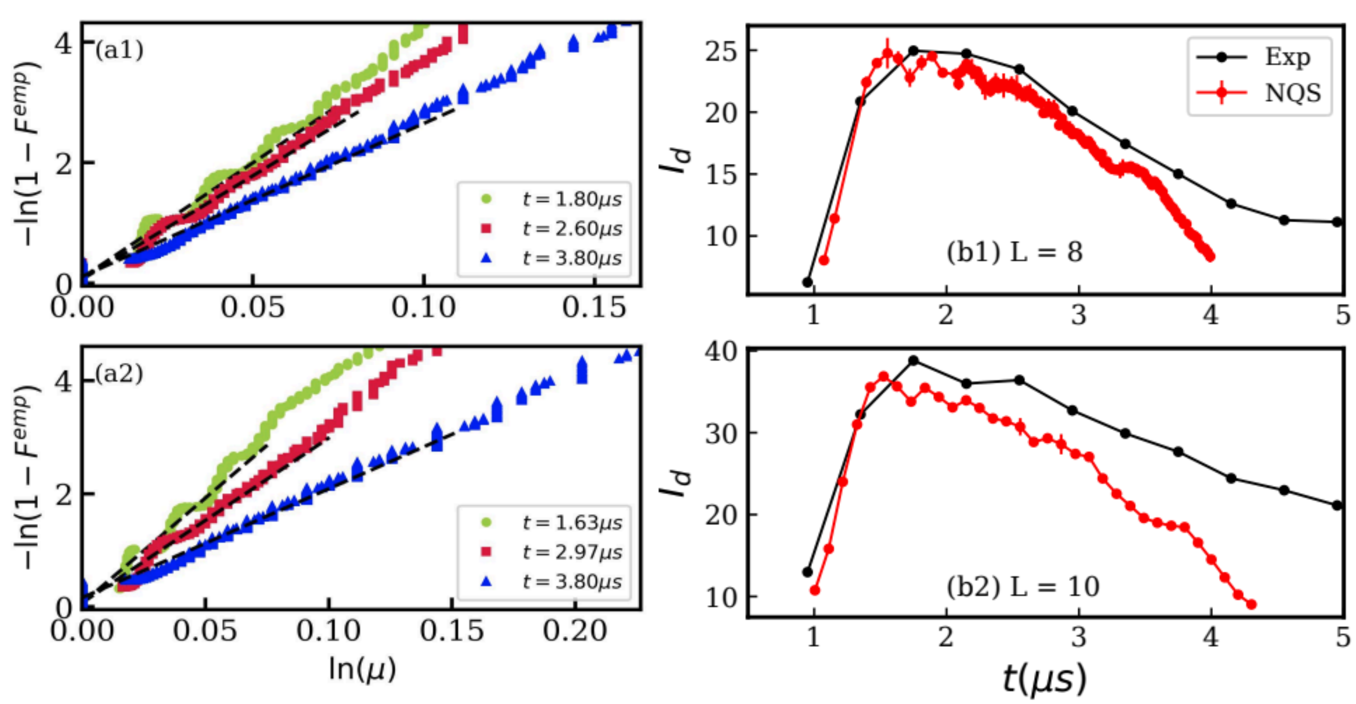
Intrinsic dimension in quantum systems



Quantum Ising chain



Mendes-Santos et al., PRX Quantum '21



Kibble-Zurek in a Rydberg quantum simulation

Mendes-Santos, Schmitt, et al., arXiv:2301.13216

Role of the physical dimension

How does volume affects the data structure and the intrinsic dimension?

3D Ising model $$E = -J \sum_{\langle i,j \rangle} S_i S_j$$

- No analytical solution known so far
- Continuous phase transition at $T_c \approx 4.51$ (believed to be conformal)
- Dual to a $\mathbb{Z}_2$ lattice gauge theory
- QCD critical point expected to belong to the 3D Ising universality class
  [Stephanov et al., PRL '98; Gavin et al., PRD '94; …]

Panda, RV, et al., arXiv:2308.13636

Volume effects on I_d: TWO-NN

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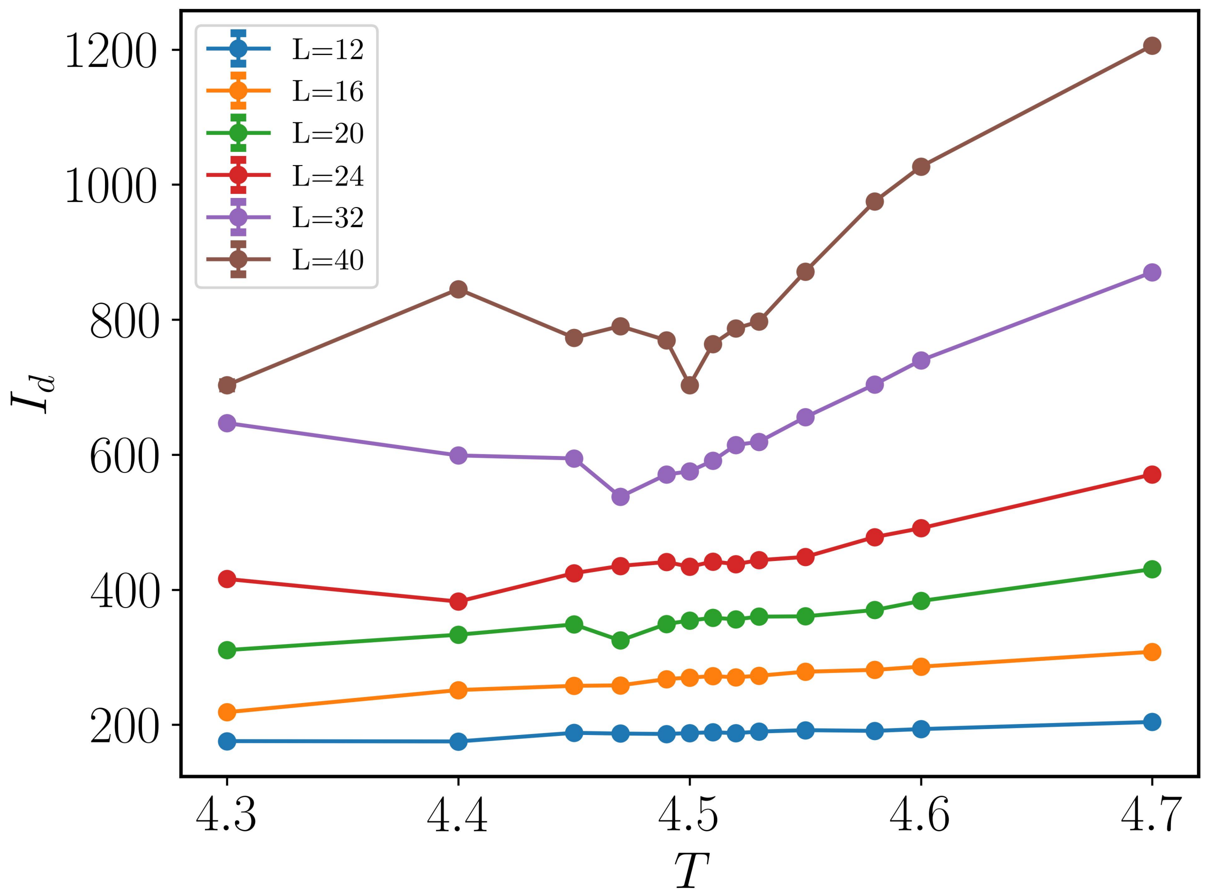

- Very high I_d (results must be taken warily)
- Minimum not so clear at the transition (TWO-NN estimator)
- In general, harder to extract information through I_d

Panda, RV, et al., arXiv:2308.13636

PCA entropy

Can we use complementary statistical tests to still be able to extract relevant information?

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Principal Component Analysis (PCA)

Transformation of the coordinate system to find high-variance directions

It amounts to diagonalizing the covariance matrix $\mathbf{\Sigma} = \mathbf{X}^T\mathbf{X}/(N_r - 1)$:

$$\mathbf{\Sigma}\lambda_n = \lambda_n \overrightarrow{w}_n$$

See e.g. Jolliffe (2005)

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See e.g. Jolliffe (2005)

Normalized eigenvalues:

$$\tilde{\lambda}_n = \frac{\lambda_n}{\sum_m \lambda_m}$$

By construction: $\tilde{\lambda}_n \geq 0, \ \sum_n \tilde{\lambda}_n = 1$

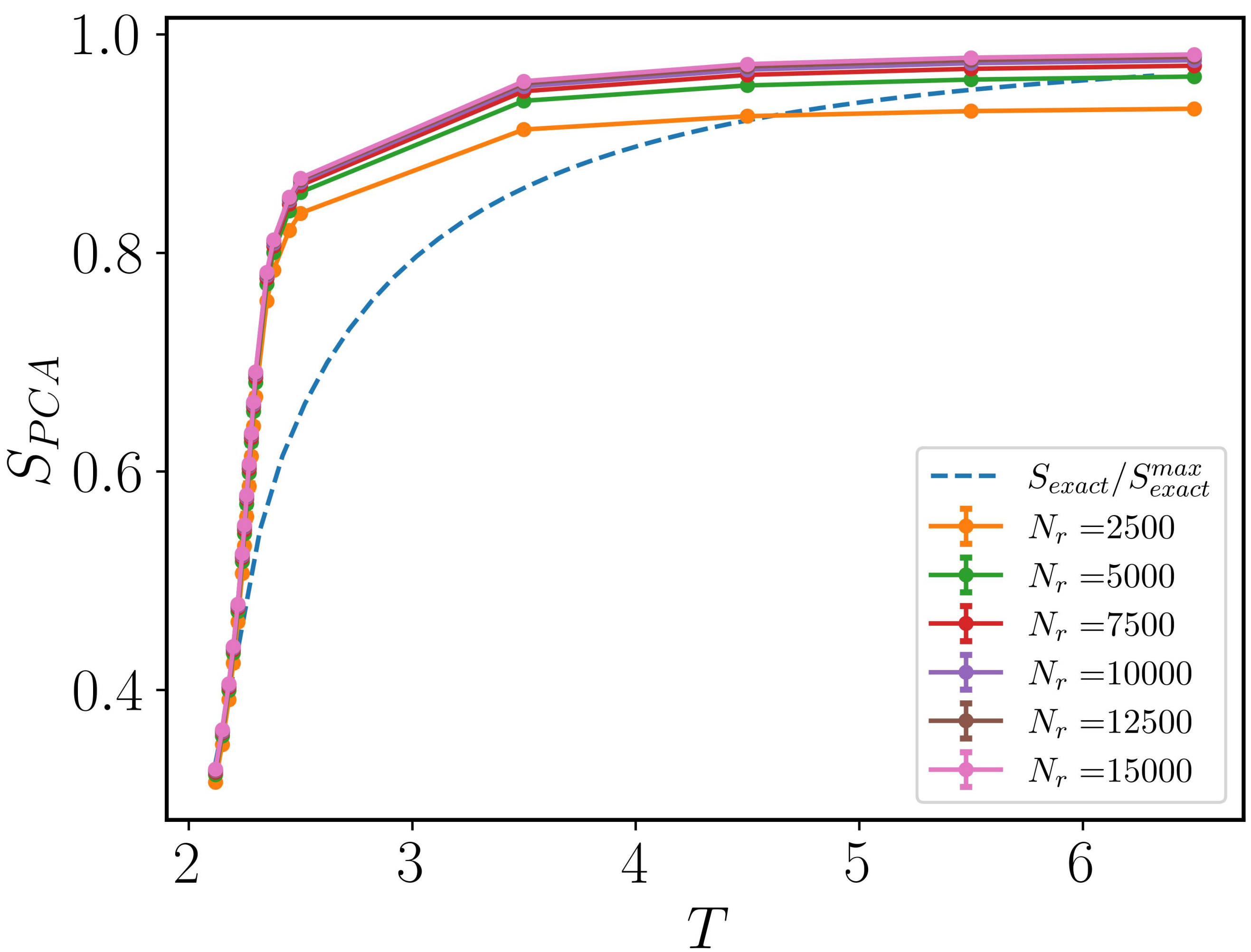
("Shannon") PCA entropy

$$S_{\mathrm{PCA}} = -\sum_n \tilde{\lambda}_n \ln(\tilde{\lambda}_n)$$

Alter et al., PNAS (2000), …

PCA entropy: 2D Ising

Striking qualitative similarity to the thermodynamic entropy!



- Suggests a direct link between the thermodynamic entropy and the (easy-to-compute) PCA entropy
- See also alternative approaches using ML or compression algorithms, eg. Nir et al., PNAS '20; Avinery et al., PRL '19; etc.

Panda, RV, et al., arXiv:2308.13636

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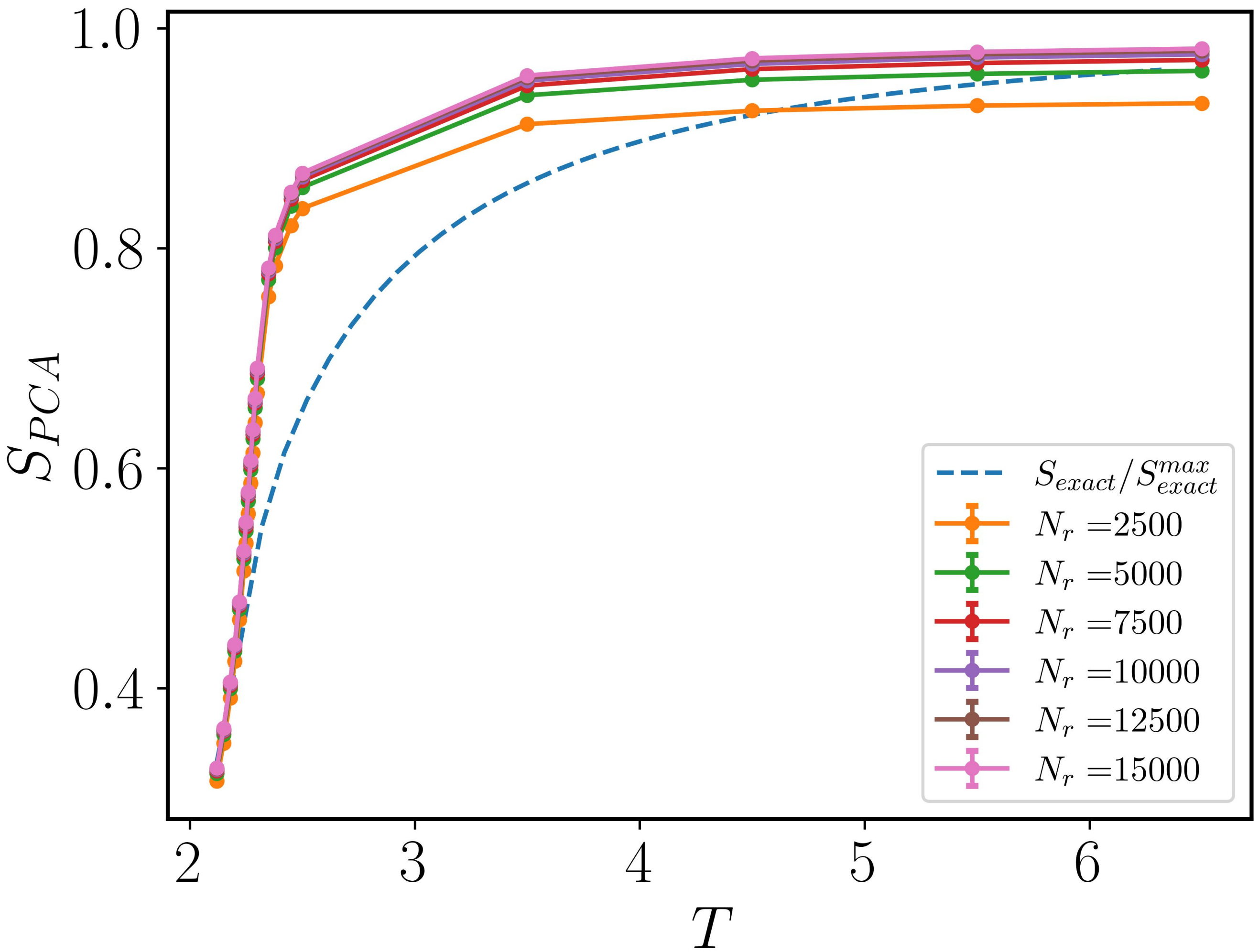
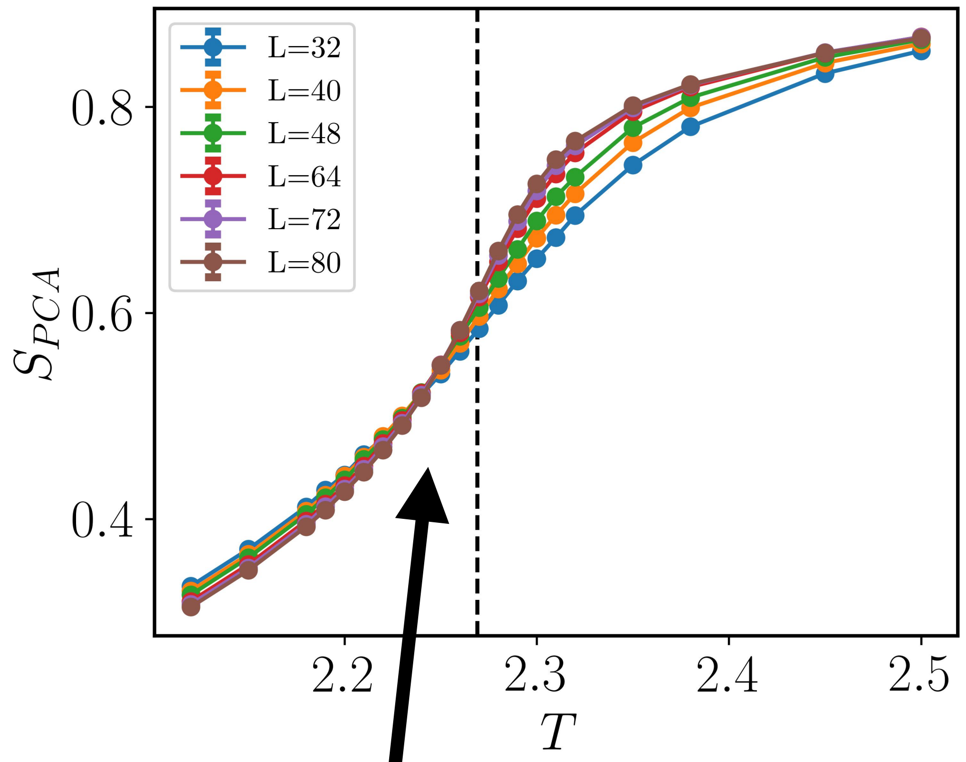


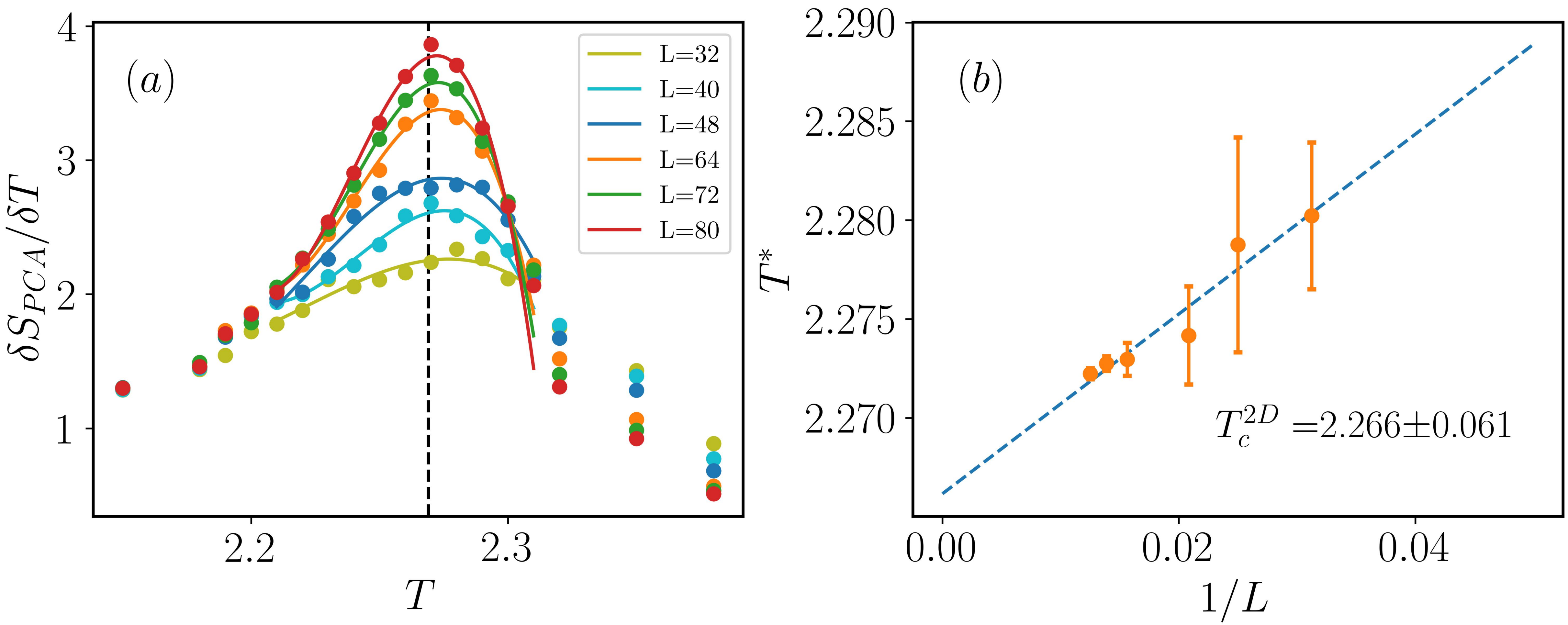


Flex very close to the transition point

Panda, RV, et al., arXiv:2308.13636

PCA entropy: 2D Ising

Quantitative prediction of T_c via a linear finite-size scaling analysis

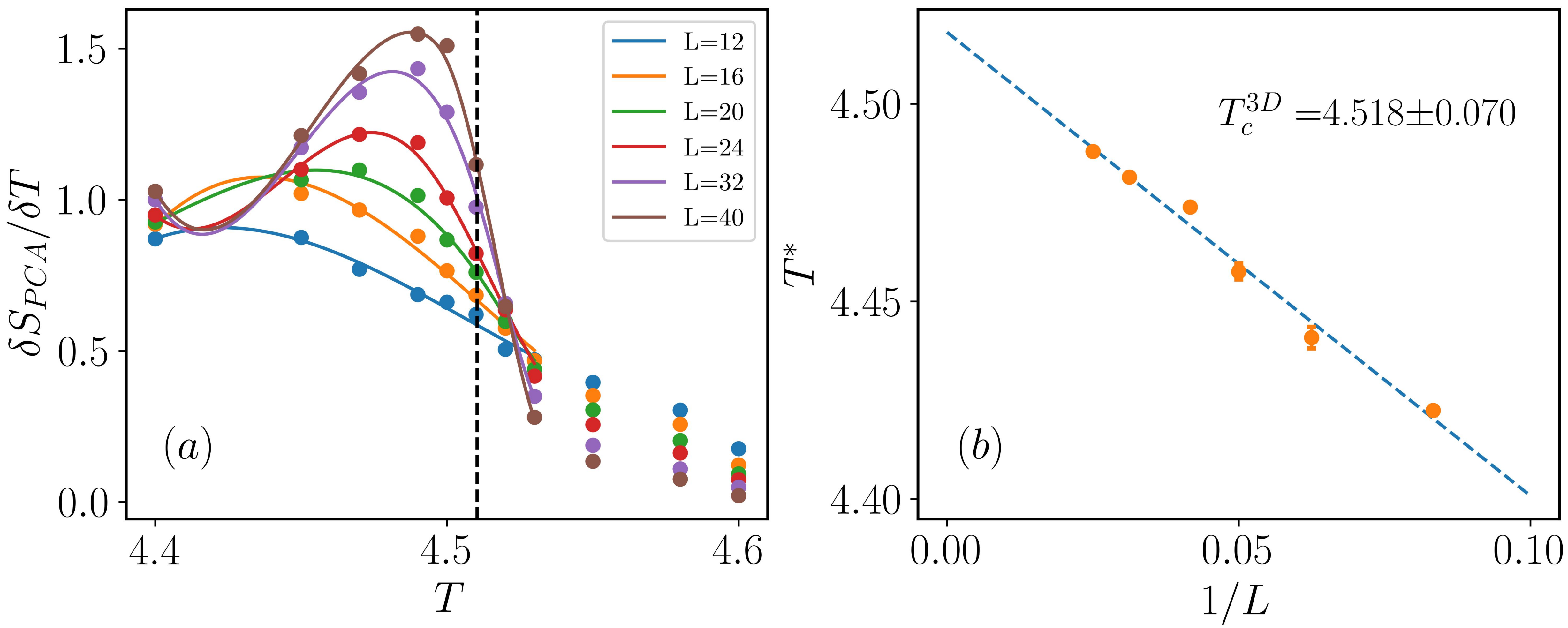


Allows to estimate T_c with less than 1% error

Panda, RV, et al., arXiv:2308.13636

PCA entropy: 3D Ising

Also works nicely for the 3D model!



Panda, RV, et al., arXiv:2308.13636

Data-driven discovery of relevant information in quantum simulation

RV et al., arXiv:2307.10040

In collaboration with M. Oberthaler's group

Experiments

LETTERS

https://doi.org/10.1038/s41567-020-0933-6

nature physics

Check for updates

Experimental extraction of the quantum effective action for a non-equilibrium many-body system

Maximilian Prüfer[1,3], Torsten V. Zache[2,3], Philipp Kunkel[1], Stefan Lannig[1], Alexis Bonnin[1], Helmut Strobel[1], Jürgen Berges[2] and Markus K. Oberthaler[1]

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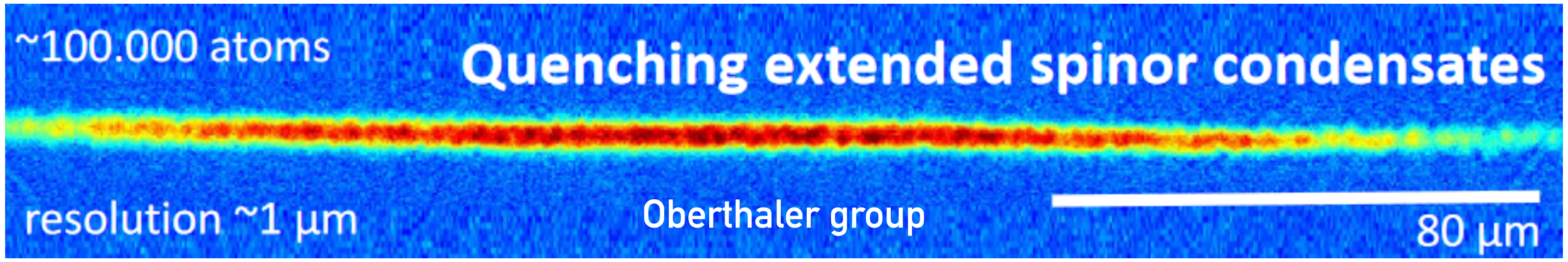

$$\Gamma_t[\Phi] = \sum_{n=1}^{\infty} \frac{1}{n!} \Gamma_t^{\alpha_1,\dots,\alpha_n}(y_1,\dots,y_n)\, \Phi^{\alpha_1}(y_1)\cdots\Phi^{\alpha_n}(y_n)$$

$\downarrow$

What are the relevant operators to determine the proper vertices?

Experiments

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Obtained from irreducible parts of correlators of the transverse spin

$$F_\perp(y) = F_x(y) + iF_y(y) = |F_\perp(y)|e^{i\varphi(y)}$$

See e.g. Kawaguchi & Ueda, Phys. Rep. '12

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$$F_\perp(y) = F_x(y) + iF_y(y) = |F_\perp(y)|e^{i\varphi(y)}$$

See e.g. Kawaguchi & Ueda, Phys. Rep. '12

Determined by particular combinations of populations

$$F_x(y) = \left(N_{+2}^{F=2}(y) - N_{-2}^{F=2}(y)\right)/N_{\mathrm{tot}}^{F=2}(y)$$

$$F_y(y) = \left(N_{+1}^{F=1}(y) - N_{-1}^{F=1}(y)\right)/N_{\mathrm{tot}}^{F=1}(y)$$

Ranking observables: PCA entropy

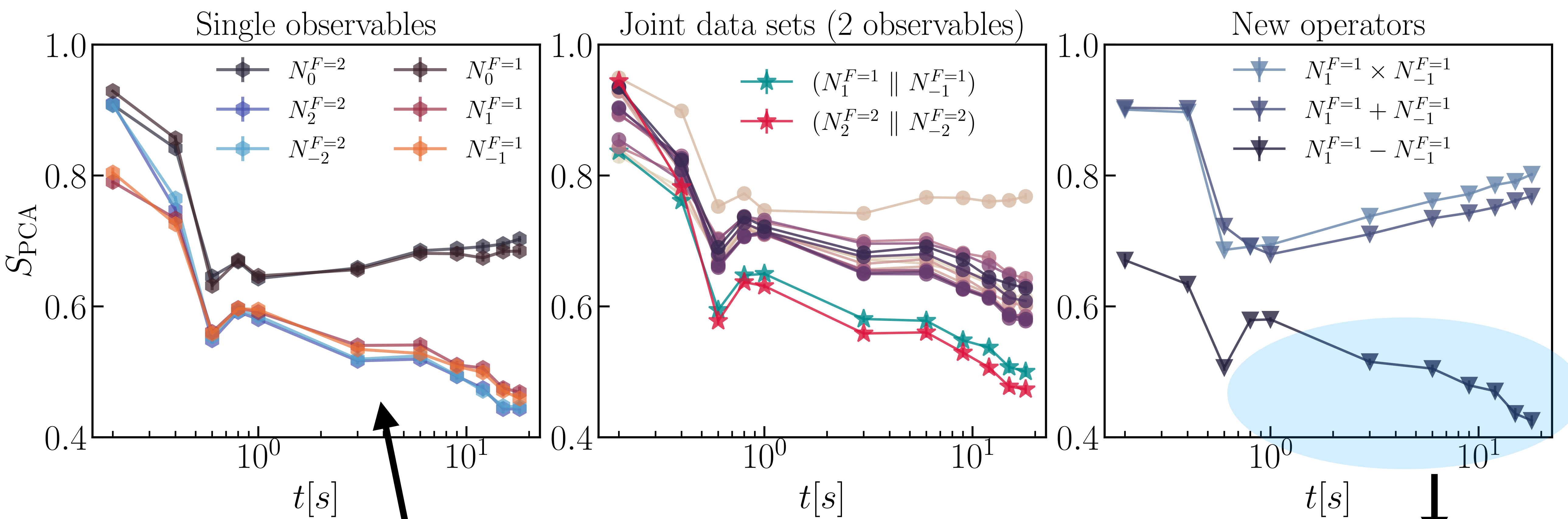
<u>Remember</u>: PCA entropy quantifies how 'messy' a data set is.

In that sense, PCA entropy can be used as a metric to rank different observations according to their relevance

The lower S_{PCA}, the stronger the correlations captured by a given observation

The higher S_{PCA}, the more 'randomness' (less predictive power)

Ranking observables: PCA entropy



The curves correspond to observations in different basis

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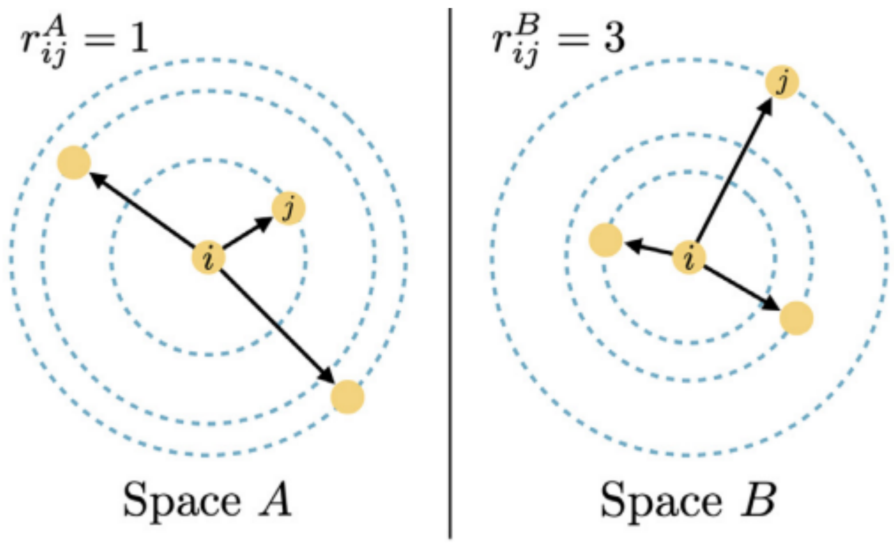
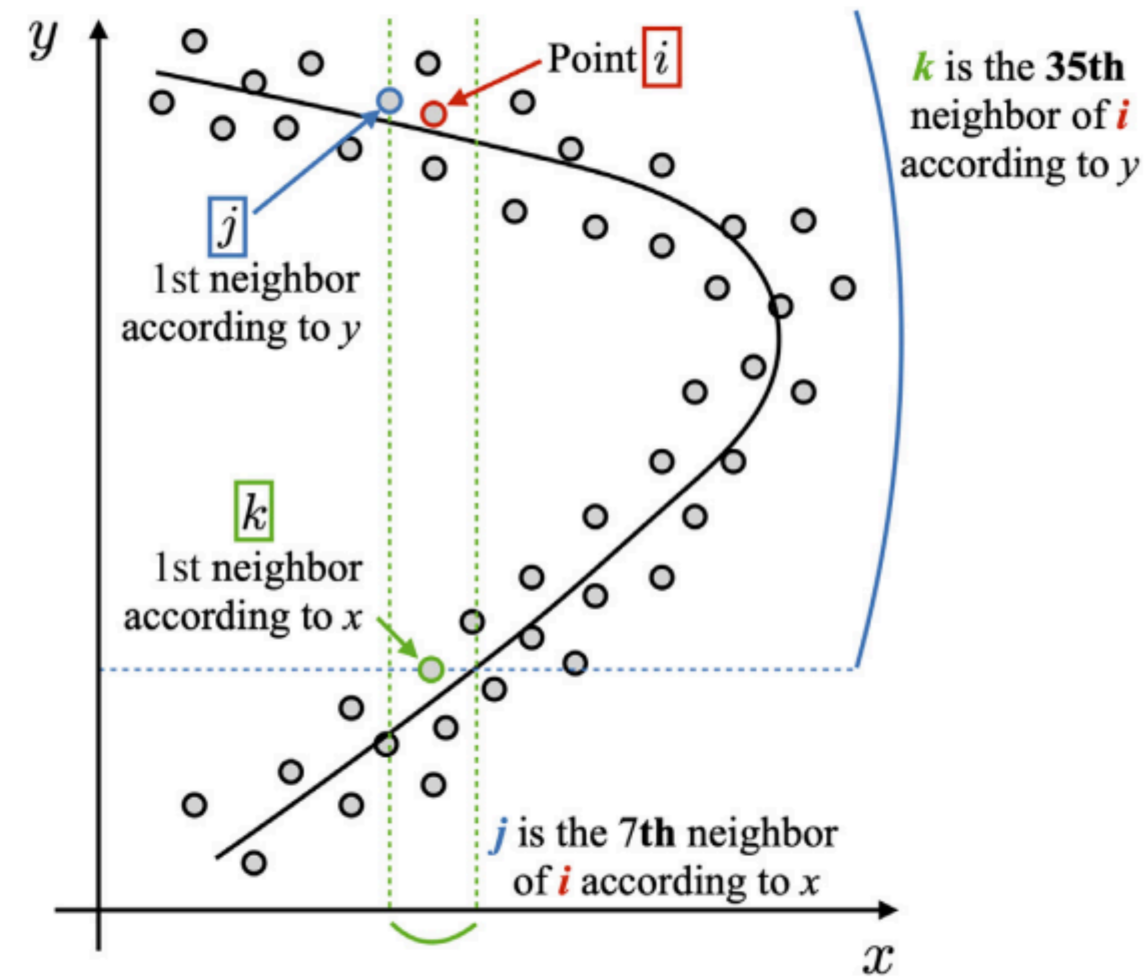
$$F_y(y) = \left(N_{+1}^{F=1}(y) - N_{-1}^{F=1}(y)\right)/N_{\mathrm{tot}}^{F=1}(y)$$

Ranking observables: information imbalance

Recently developed ML technique to quantify the relative amount of information between different types of variables

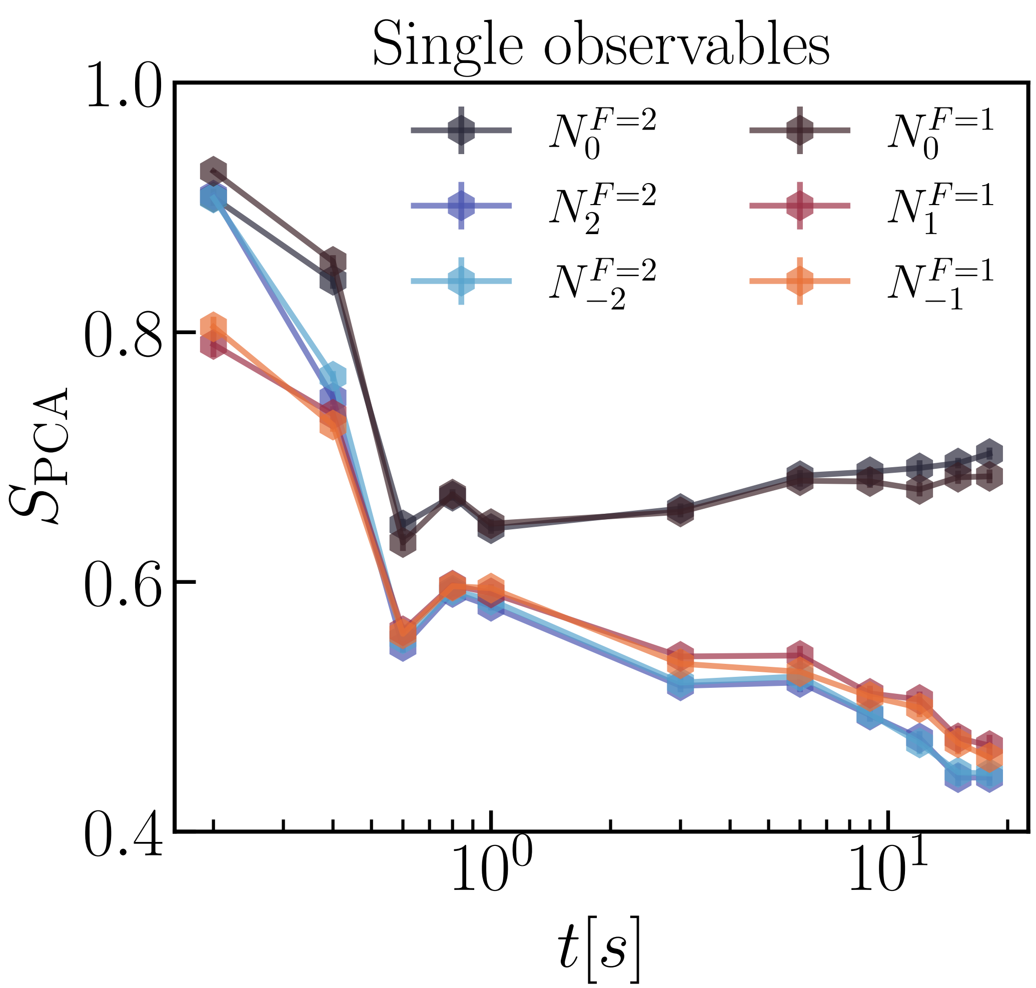


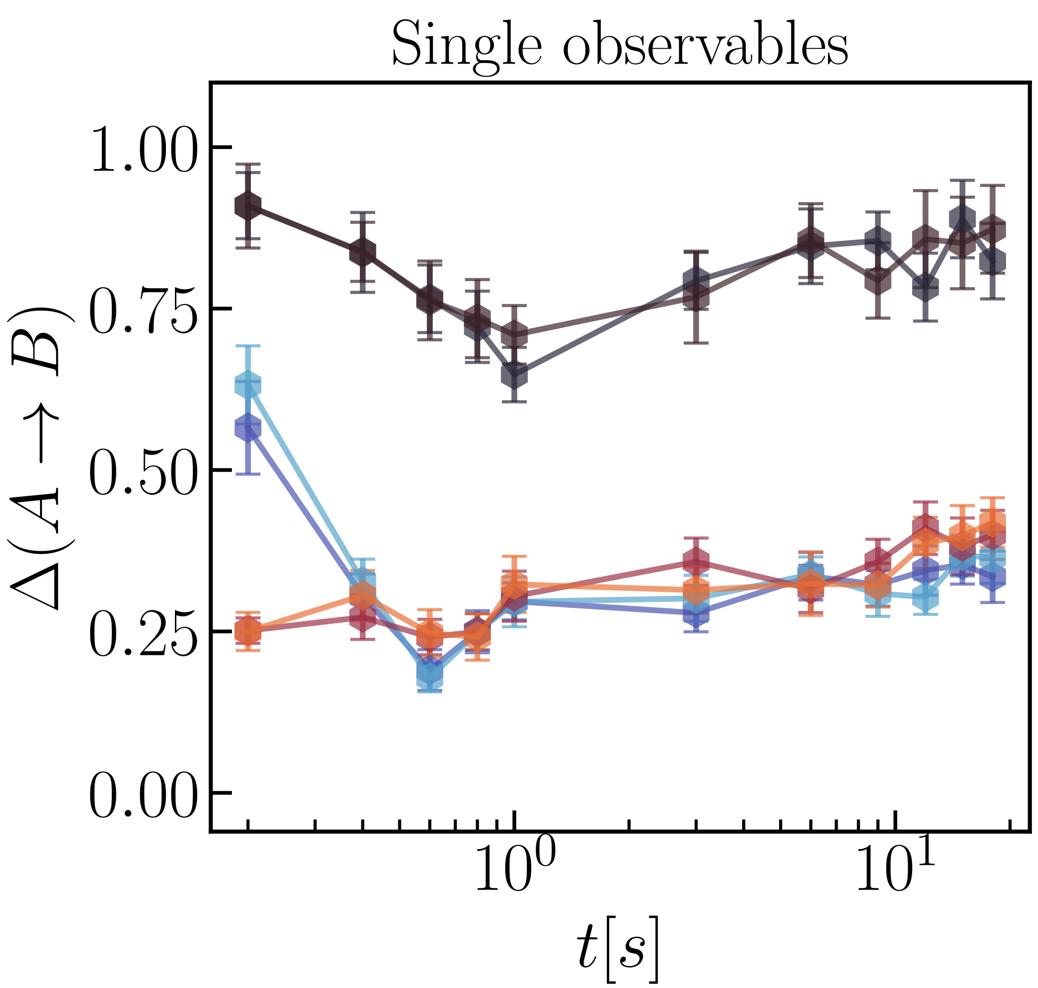
$$\Delta(A \to B) = \frac{2}{N_r^2} \sum_{i,j:r_{ij}^A=1} r_{ij}^B$$



Glielmo et al., PNAS Nexus '22

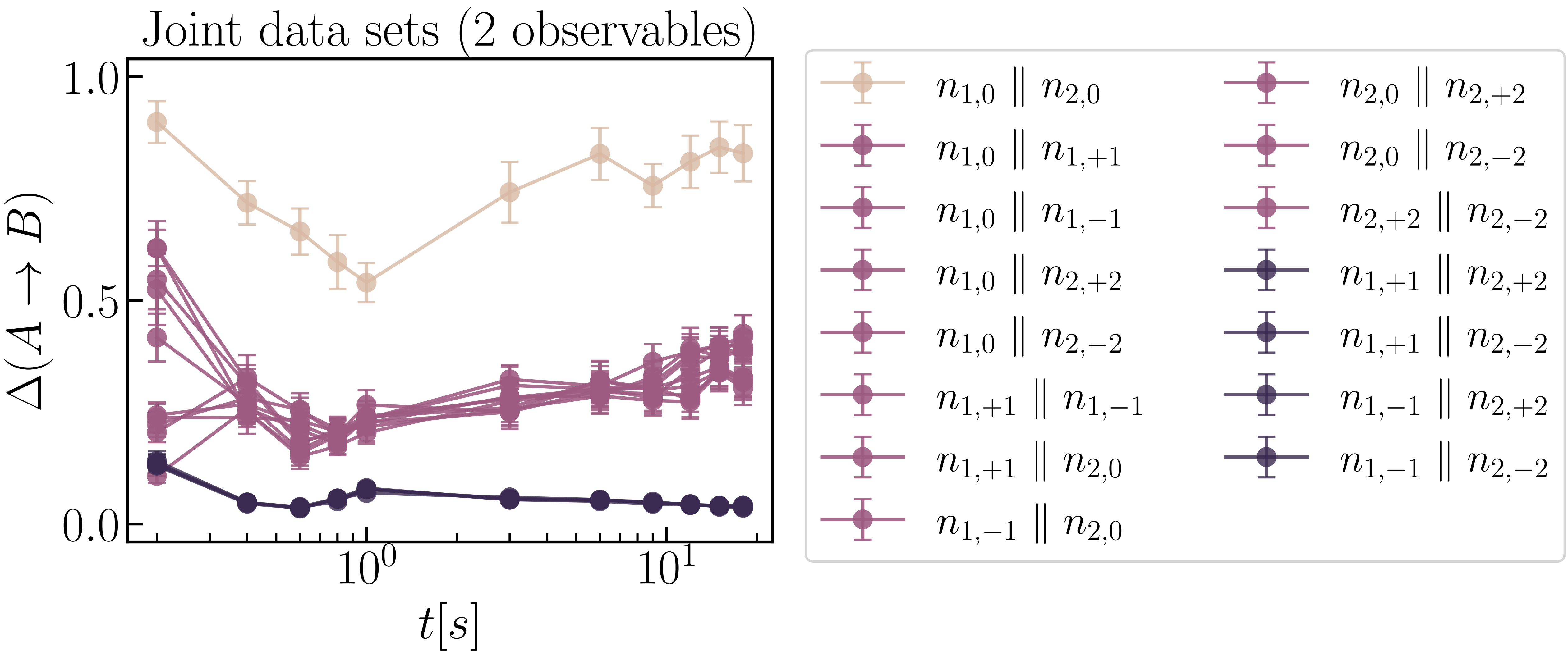
Ranking observables: information imbalance





Cross-verifies ranking obtained with PCA entropy

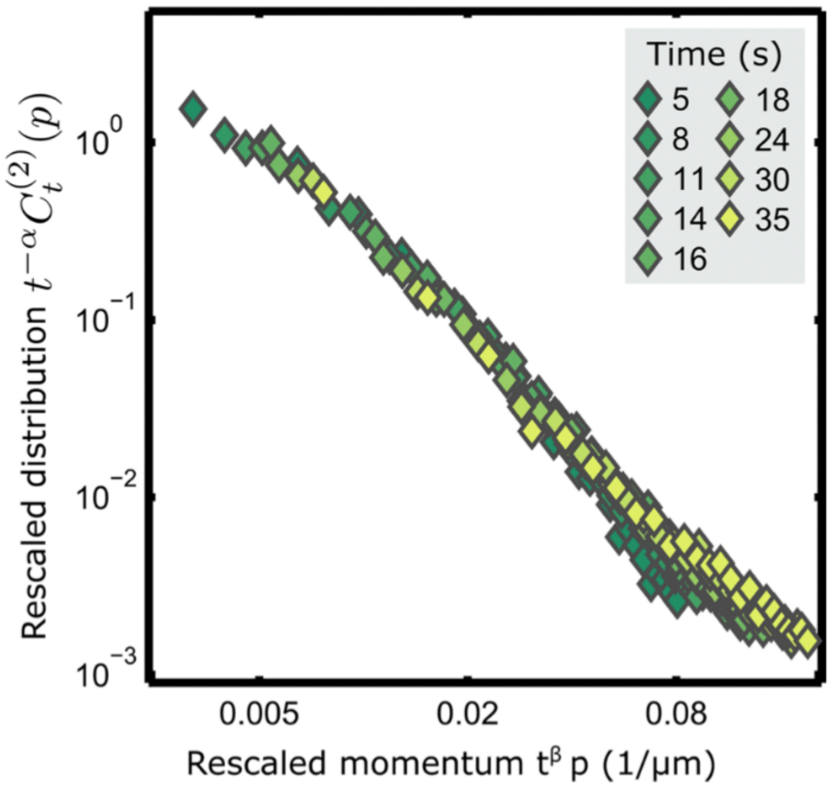
Ranking observables: information imbalance



Complementary characterisation of relevance: needs to combine observables from two relevant pairs to describe the full space of observations

Agnostic bound on universal scaling regime

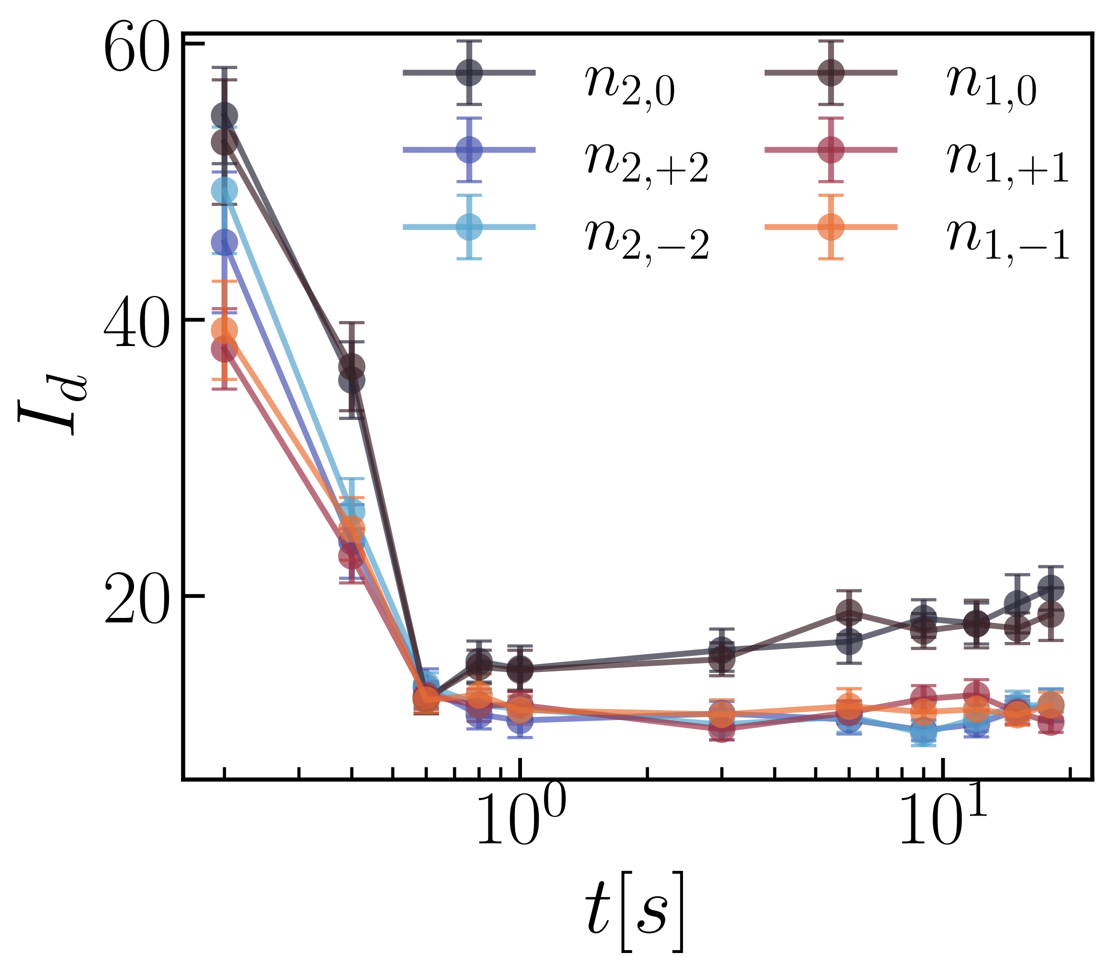
Correlation functions of the transverse spin exhibit self-similar dynamics



Prüfer et al., Nat. Phys. '20

Theo: Berges et al., PRL '08, …

Intrinsic dimension features long, stable plateaus in strong agreement with universal behavior



Conclusions and Outlook

- Non-parametric unsupervised methods provide powerful tools to enable assumption-free discoveries in many-body physics!
- Widely applicable methods: classical/quantum, in and out of equilibrium, and working with limited sampling
- Insights on lattice gauge theory and topological matter (on-going)
- Interesting connections to the entropy and measures of complexity (e.g. Kolmogorov complexity, Shannon entropy)

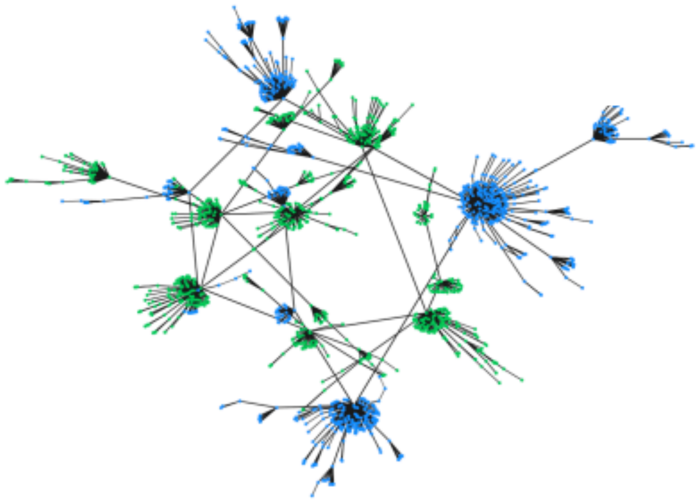
Thank you!

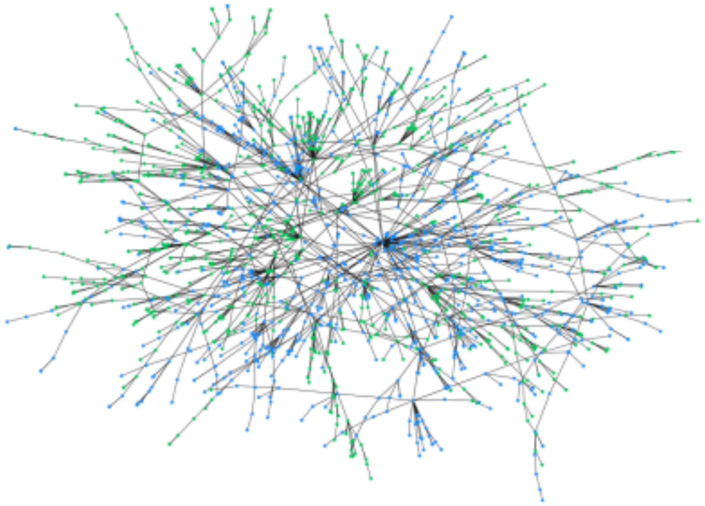
What I didn't talk about

Complex network based 'data mining'

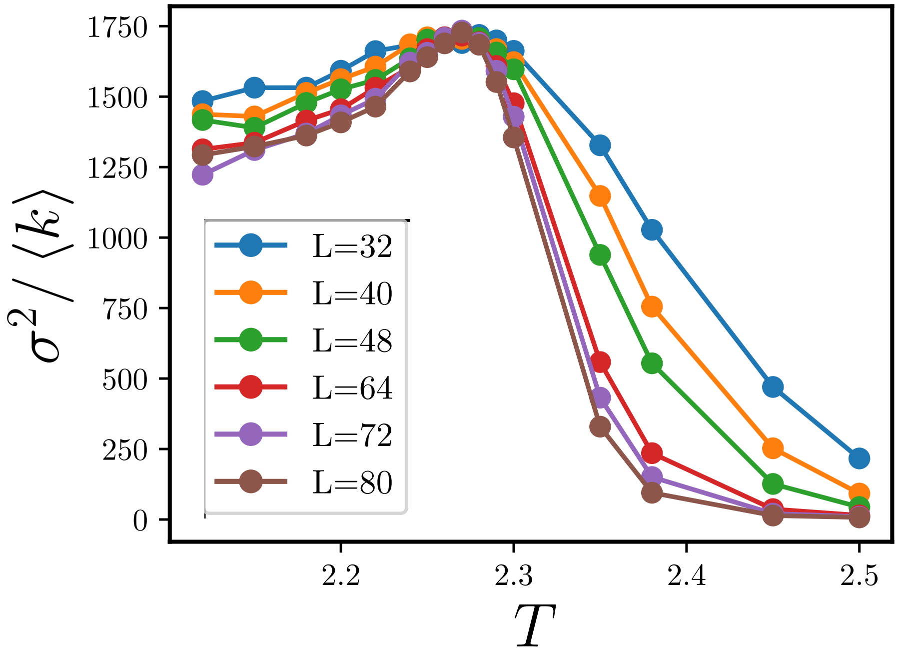
H. Sun

G. Bianconi





- Plethora of tools from network science that provide an in-depth statistical, combinatorial, geometrical and topological analysis of data sets
- Nice complementary tools for unsupervised approaches



Sun, RV, et al., arXiv:2308.13604 (see also arXiv:2301:13216)

Extra material

More about intrinsic dimension

- Lower bound of complexity in data sets (e.g. relation to bottleneck in autoencoders [Ansuini et al., NearIPS 2019])
- Crucial dependence on the chosen scale

Mendes-Santos et al., PRX '21

- Related to the Kolmogorov complexity

How long shall a classical computer code be to reproduce a given string?

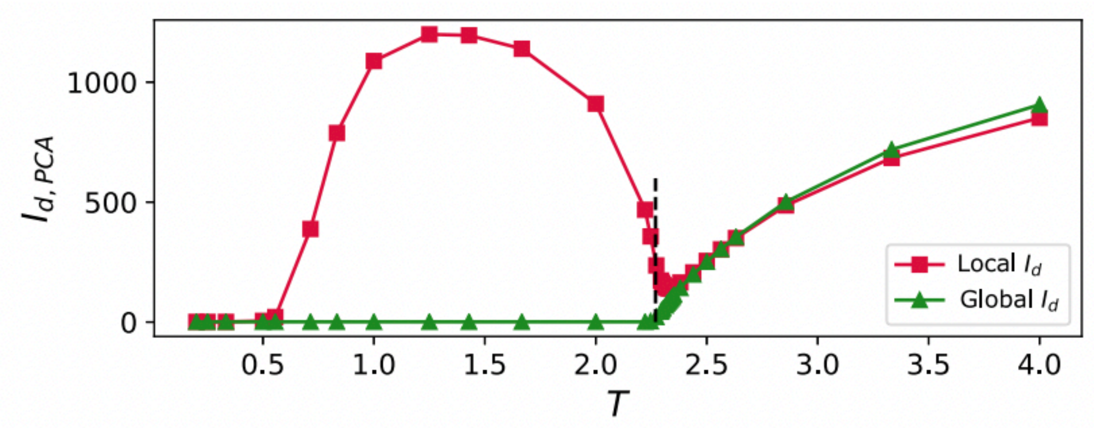
'11111111…'	'10011010…'
print '1' n times (lower complexity)	print '10011010…' (higher complexity)

I_d estimation: PCA

See e.g. Jolliffe (2005)

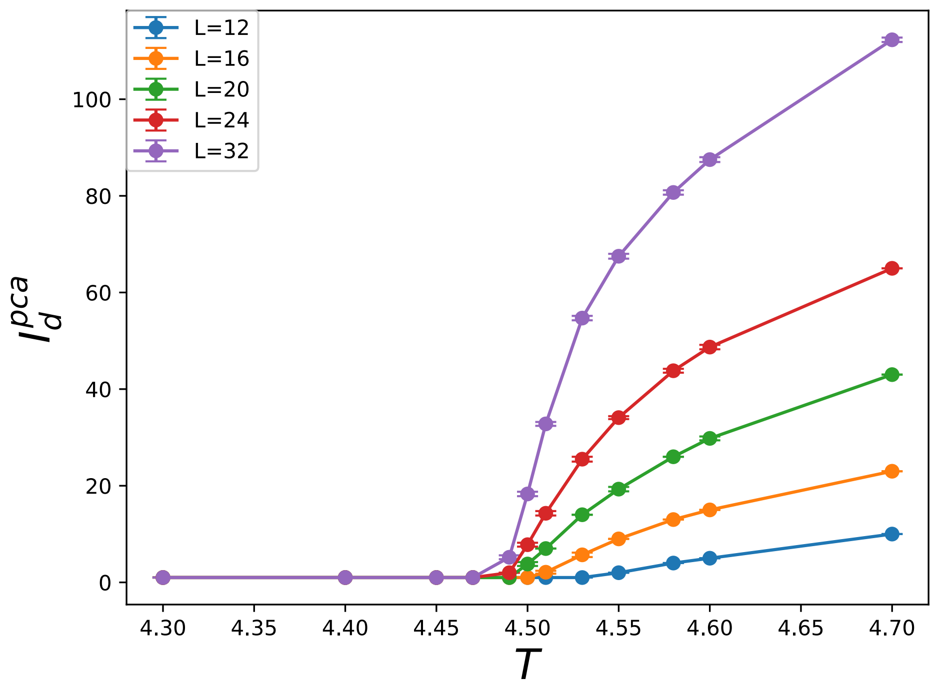
- Based on a ad-hoc cutoff parameter in the integrated spectrum of the covariance matrix $\sum_{n=1}^{I_d} \tilde{\lambda}_n \approx \zeta$
- Bad estimate for curved manifolds

2D Ising



Mendes-Santos et al., PRX '21

3D Ising



Panda, RV, et al., arXiv:2308.13636