

QCD相变的神经网络解析和数据几何

NN Analysis of QCD Phase Transition & Data Geometry



汇报人：梅杰

合作者：黄梅 教授 (UCAS)、王凌霄 (Riken, iTHEMS)

Outline

- 机器学习简介
- 通过神经网络提取胶子的色电与色磁质量
- 基于内禀维数的新型退禁闭判据研究

机器学习方法简介

概率视角

从**数据**中学习**潜在分布**,

$$\mathbf{x} = (x_1, x_2, \dots, x_N)$$

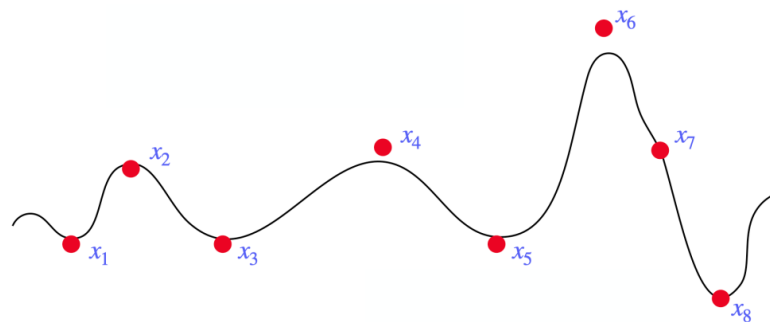
监督学习, $p_{\text{data}}(\mathbf{y} | \mathbf{x})$

非监督学习, $p_{\text{data}}(\mathbf{x})$

网络参数 $\{\theta\}$

$$\max_{\theta} \prod_{i=1}^N p_{\theta}(\mathbf{x}_i)$$

$$\mathbf{x} \sim p_{\text{data}}(\mathbf{x})$$



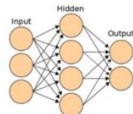
Maximum likelihood estimation(MLE)

机器学习方法简介

监督学习

FLUCTUATIONS HANDWRITTEN DIGITS (MNIST)

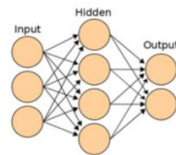
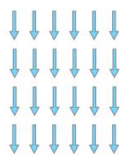
0 0 0 0 0 0 0 0 0 0 0 0
1 1 1 1 1 1 1 1 1 1 1 1
2 2 2 2 2 2 2 2 2 2 2 2
3 3 3 3 3 3 3 3 3 3 3 3
4 4 4 4 4 4 4 4 4 4 4 4
5 5 5 5 5 5 5 5 5 5 5 5
6 6 6 6 6 6 6 6 6 6 6 6
7 7 7 7 7 7 7 7 7 7 7 7
8 8 8 8 8 8 8 8 8 8 8 8
9 9 9 9 9 9 9 9 9 9 9 9



ML community has developed
powerful **supervised** learning
algorithms

$\mathcal{S} = 5 + \text{fluctuations}$

FM phase

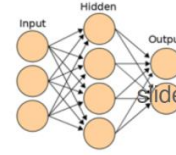
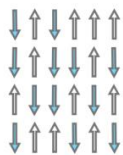


FM (0)

High T phase



gray=spin up
white=spin down



PM (1)

J. Carrasquilla and R. G. Melko. Nature Physics 13, 431–434 (2017)

机器学习方法简介

监督学习

FLUCTUATIONS HANDWRITTEN DIGITS (MNIST)

0000000000000000
1111111111111111
2222222222222222
3333333333333333
4444444444444444
5555555555555555
6666666666666666
7777777777777777
8888888888888888
9999999999999999

$\mathcal{S} = 5 + \text{fluc}$

FM pha

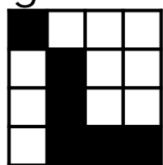


High T ph

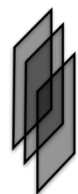


Convolutional neural net as a “thermometer”

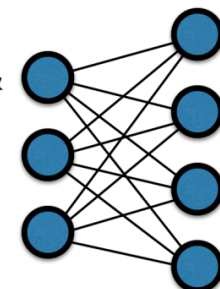
Ising conf. at β



*



Flatten & Input



Output β_{CNN}

Ans. β

$$-\sum_{l=1}^N \beta_l \log \beta_l^{\text{CNN}},$$

10^2 confs.
for each β

Conv. w/
3 filters

Fully con. NN
 W

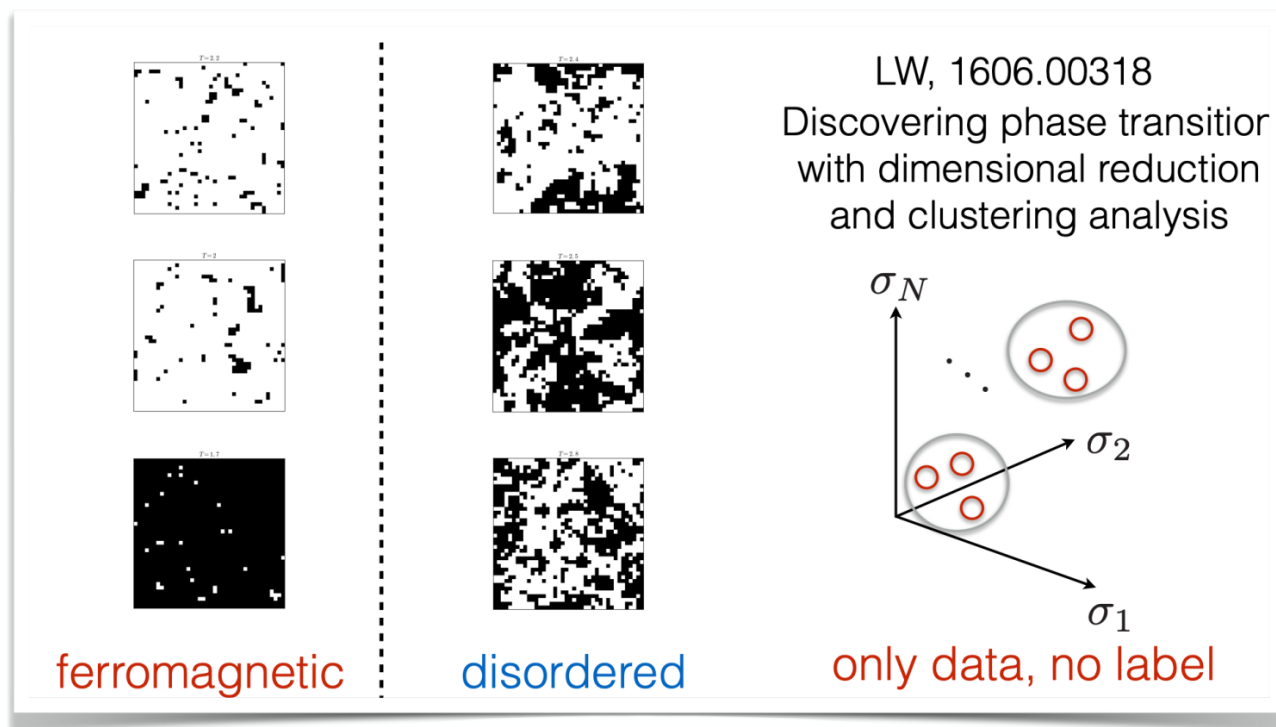
Inv. β is
discretized for
labeling
(one-hot)

$$\vec{\beta} = \begin{cases} (1, 0, \dots, 0, 0) & \text{for } \beta < 0 \\ (0, 1, \dots, 0, 0) & \text{for } \beta \in \left[0, \frac{1}{N-2}\right) \\ \dots & \\ (0, 0, \dots, 1, 0) & \text{for } \beta \in \left[\frac{N-3}{N-2}, 1\right) \\ (0, 0, \dots, 0, 1) & \text{for } 1 \leq \beta \end{cases} \quad \begin{matrix} 0.2 < \beta < 10, \\ \\ \\ \\ N = 100 \end{matrix}$$

Akinori Tanaka, and Akio Tomiya, *J. Phys. Soc. Jpn.* 86, 063001 (2017)

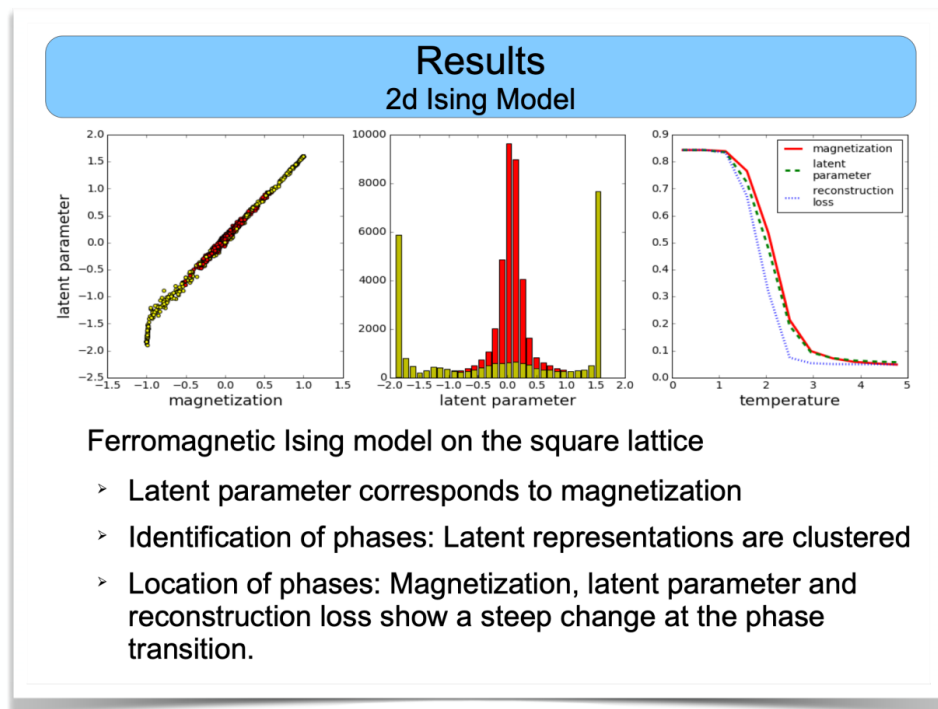
机器学习方法简介

非监督学习

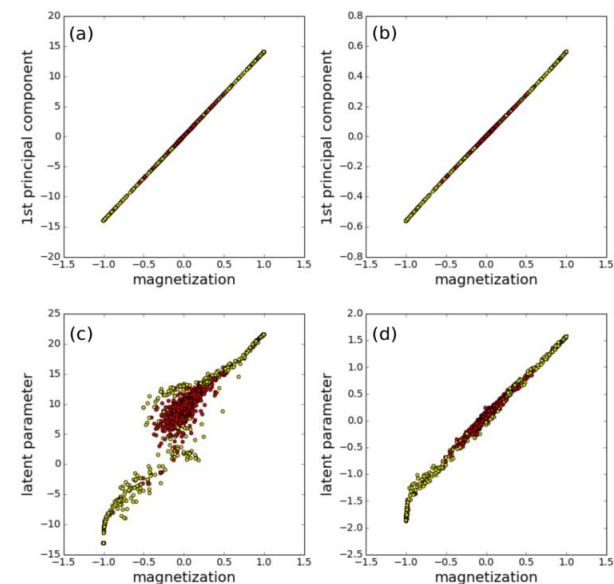


机器学习方法简介

非监督学习



Sebastian Johann Wetzel, Phys. Rev. E 96, 022140 (2017)

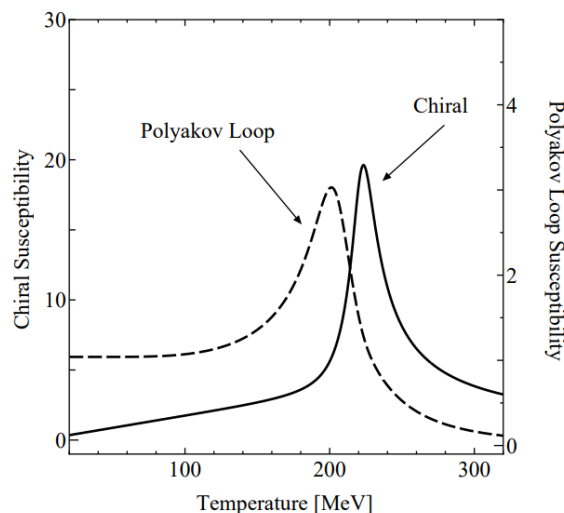
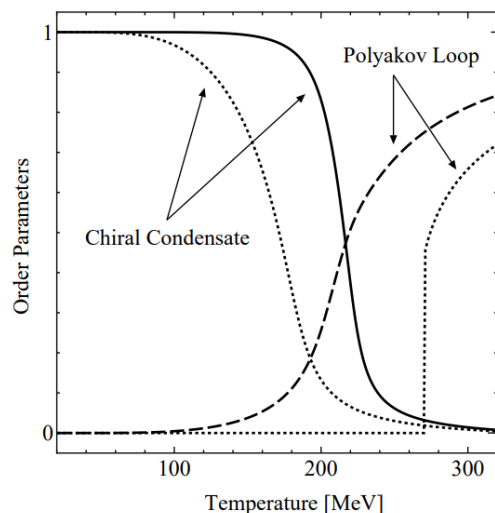


- ▶ (a) PCA
- ▶ (b) Kernel PCA
- ▶ (c) AutoEncoder
- ▶ (d) Variational AutoEncoder

通过神经网络提取色电和色磁胶子质量

研究动机

- 大量有效模型 (如NJL模型、QM模型等), 仅能描述手征恢复相变。
- 若要考虑退禁闭相变, 则需要引入Polyakov圈^圈的贡献。



Kenji Fukushima, (2004)

$$L(\vec{x}) = \mathcal{T} \exp \left[-i \int_0^\beta dx_4 A_4(x_4, \vec{x}) \right]$$

通过神经网络提取色电和色磁胶子质量

研究动机

Polyakov势
$$V(\ell) = -\frac{1}{2}a(T)\ell\bar{\ell} + b(T)\ln[1 - 6\ell\bar{\ell} + 4(\ell^3 + \bar{\ell}^3) - 3(\ell\bar{\ell})^2]$$

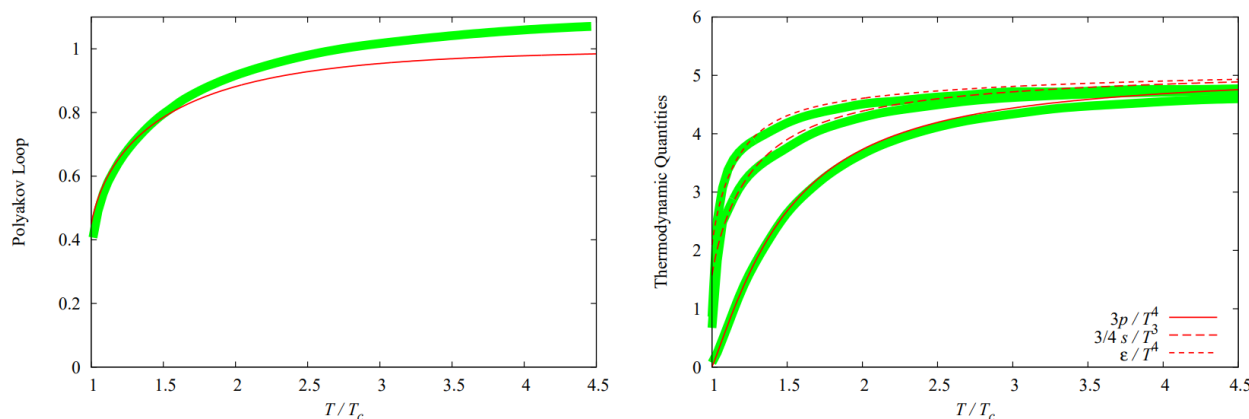


Figure 2: Comparison between the quenched lattice data (green thick curves) and the results from the potential ansatz (red thin curves). The left shows the Polyakov loop and the right shows the thermodynamic quantities.

Quenched lattice data: 色电+色磁

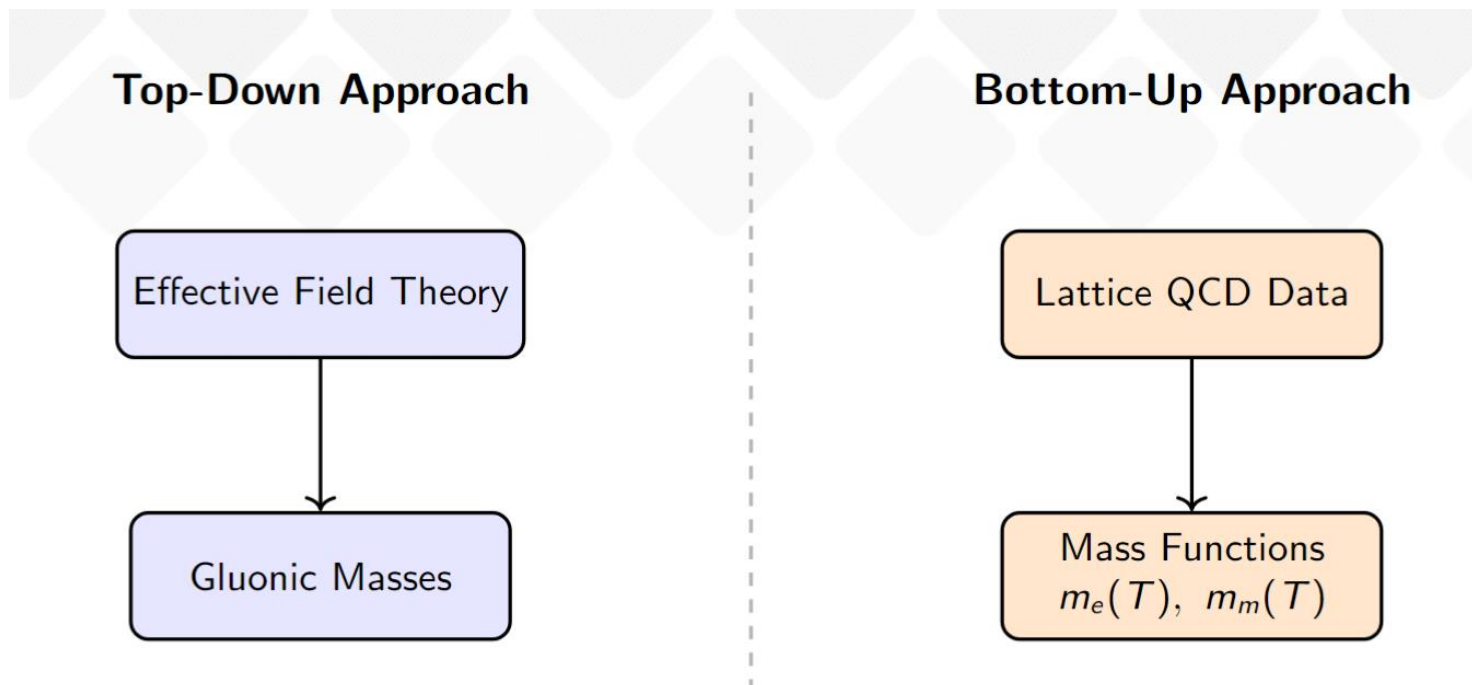
Polyakov势: 仅色电



Kenji Fukushima, (2009)

通过神经网络提取色电和色磁胶子质量

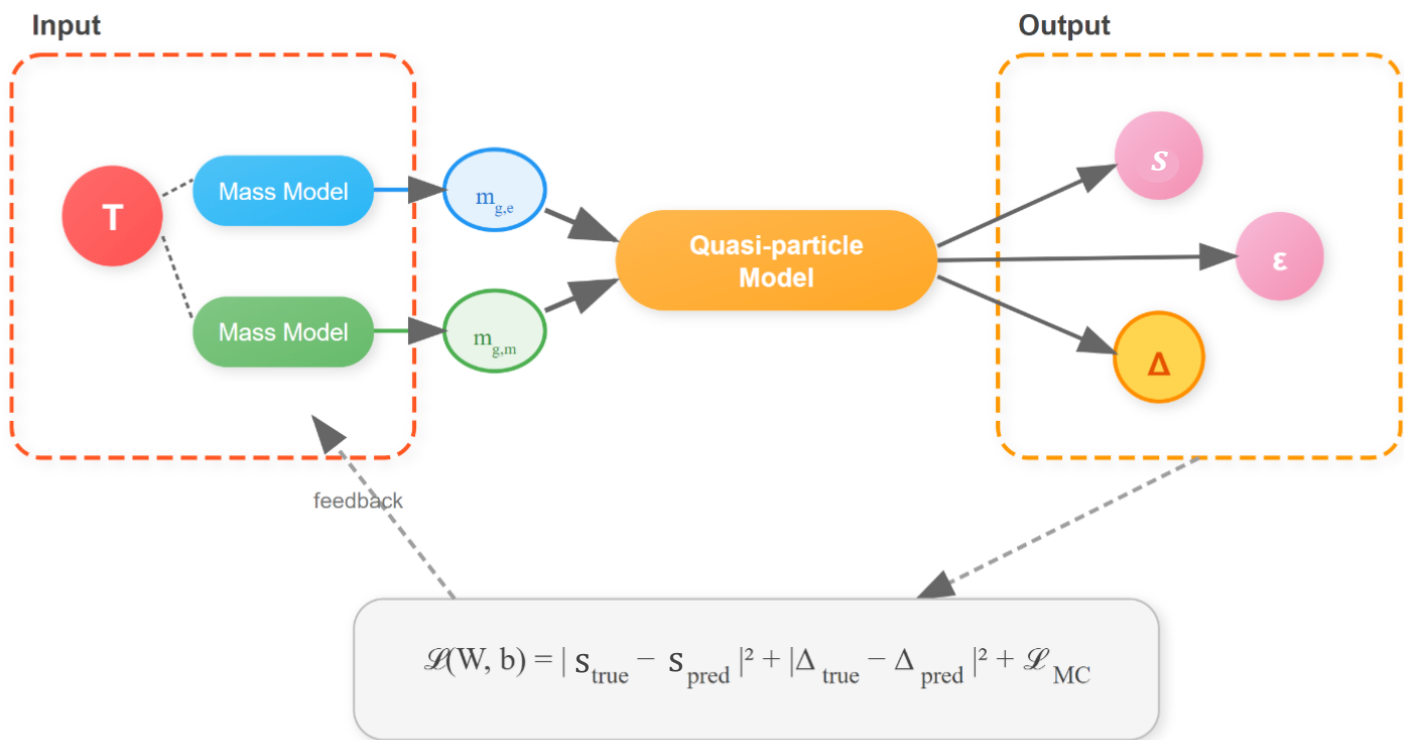
研究方法



数据驱动：直接通过格点数据约束得到胶子质量函数

通过神经网络提取色电和色磁胶子质量

研究方法



通过神经网络提取色电和色磁胶子质量

研究方法

准粒子模型中，胶子等离子体被视作有质量准粒子构成的自由气体：

$$\ln Z(T) = \ln Z_E(T) + \ln Z_M(T)$$

其中各分量服从玻尔兹曼分布

$$\ln Z_i(T) = -\frac{d_{g_i} V}{2\pi^2} \int_0^\infty dp p^2 \ln \left[1 - \exp \left(-\frac{1}{T} \sqrt{p^2 + m_{g_i}^2(T)} \right) \right]$$

m_{g_i} 为对应胶子的热质量，使用神经网络表示： $m_{g_i}(T, \theta)$

色电扇区对应胶子的纵向极化，自由度为 $d_E = 1 \times 8 = 8$ ；色磁扇区对应横向极化，自由度为 $d_M = 2 \times 8 = 16$ 。

通过神经网络提取色电和色磁胶子质量

热力学量

$$\begin{aligned} P(T) &= T \left(\frac{\partial \ln Z(T)}{\partial V} \right)_T \\ &= - \sum_{i=e,m} \frac{d_{g_i} T}{2\pi^2} \int_0^\infty dp \, p^2 \ln \left[1 - \exp \left(-\frac{1}{T} \sqrt{p^2 + m_{g_i}^2(T)} \right) \right], \\ \varepsilon(T) &= \frac{T^2}{V} \left(\frac{\partial \ln Z(T)}{\partial T} \right)_V \\ &= \sum_{i=e,m} \frac{d_{g_i} T}{2\pi^2} \int_0^\infty dp \, p^2 \left\{ \frac{\sqrt{p^2 + m_{g_i}^2(T)}}{\exp \left(\sqrt{p^2 + m_{g_i}^2(T)}/T \right) - 1} - \frac{T}{\sqrt{p^2 + m_{g_i}^2(T)}} \frac{m_{g_i}(T) (\partial m_{g_i}(T)/\partial T)}{\exp \left(\sqrt{p^2 + m_{g_i}^2(T)}/T \right) - 1} \right\}. \\ &= \varepsilon_{id}(T) + B(T) \end{aligned}$$

为了满足热力学一致性 $sT = p + \varepsilon$, 压强重写为

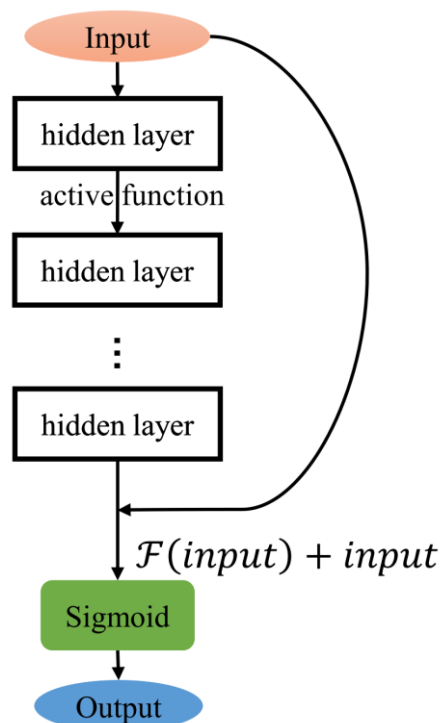
$$P(T) \rightarrow P_{id}(T) - B(T)$$

$$\text{熵: } s(T) = \frac{P(T) + \varepsilon(T)}{T} \qquad \text{迹反常: } \Delta(T) = \frac{\varepsilon(T) - 3P(T)}{T^4}$$

通过神经网络提取色电和色磁胶子质量

神经网络架构

- **Input Layer:** Maps the single input (temperature T) to a 24-dimensional hidden layer.
- **Residual Blocks:** Contains 4 residual blocks, each consisting of two linear layers with a *Swish-like* activation function in between, defined as $f(x) = x \cdot \sigma(x)$, where $\sigma(x)$ is the sigmoid function. The residual connection is achieved by adding the input directly to the block's output.
- **End Layer:** Further processes the output of the residual blocks, maintaining a hidden dimension of 24.
- **Output Layer:** Generates non-negative mass predictions using the *Softplus* activation function ($f(x) = \ln(1 + e^x)$), which guarantees the positive definiteness of gluonic masses.



残差网络 (ResNet): 在网络层数较深时有效避免梯度爆炸/消失问题

通过神经网络提取色电和色磁胶子质量

损失函数

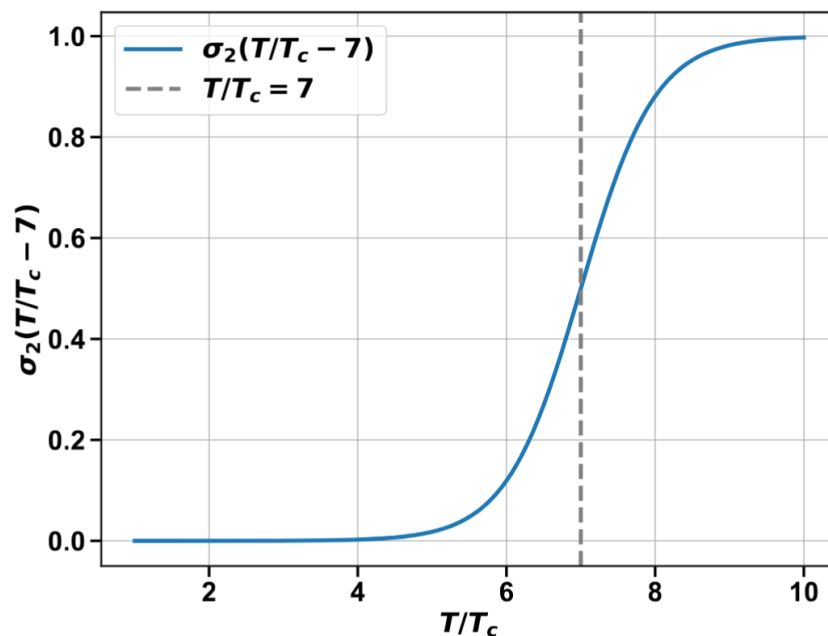
$$\mathcal{L} = \mathcal{L}_{\text{MSE}} + \mathcal{L}_{\text{MC}}$$

均方误差 (MSE): 训练预测值与格点真实值之间的差别

$$\mathcal{L}_{\text{MSE}} = \text{MSE}(s_{\text{pred}}/T^3, s_{\text{true}}/T^3) \\ + \text{MSE}(\Delta_{\text{pred}}, \Delta_{\text{true}})$$

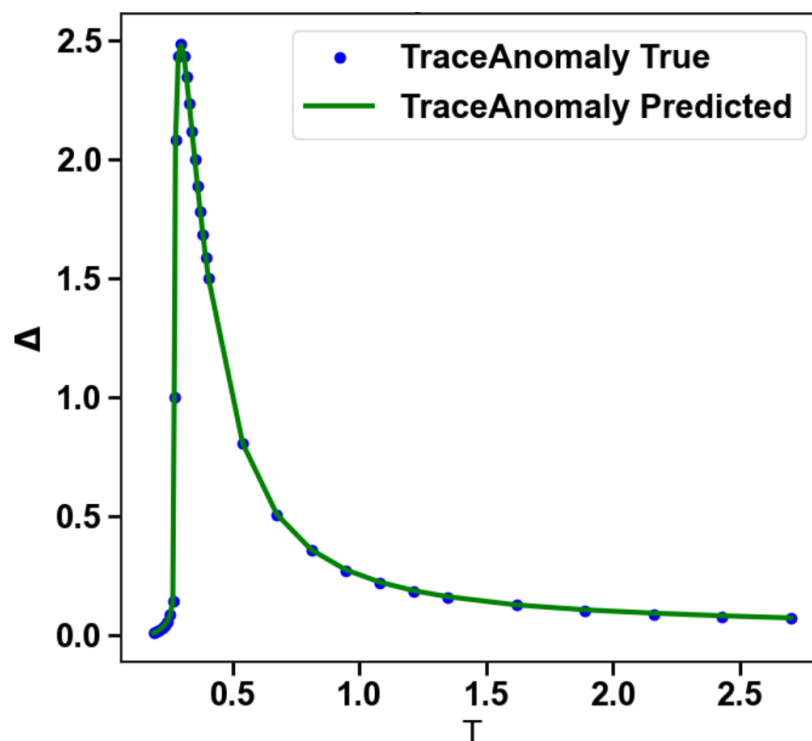
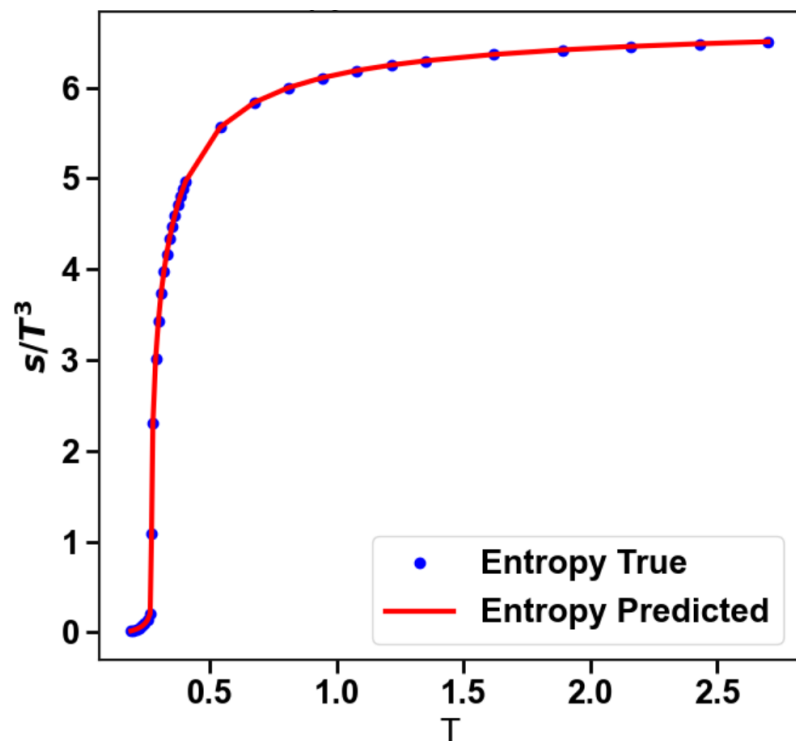
正则项: 高温时, 色磁部分质量趋近微扰QCD结果

$$\mathcal{L}_{\text{MSE}} = \omega(T) \left[m_M(T) - \frac{1}{\sqrt{2}} g(T) T \right]^2$$



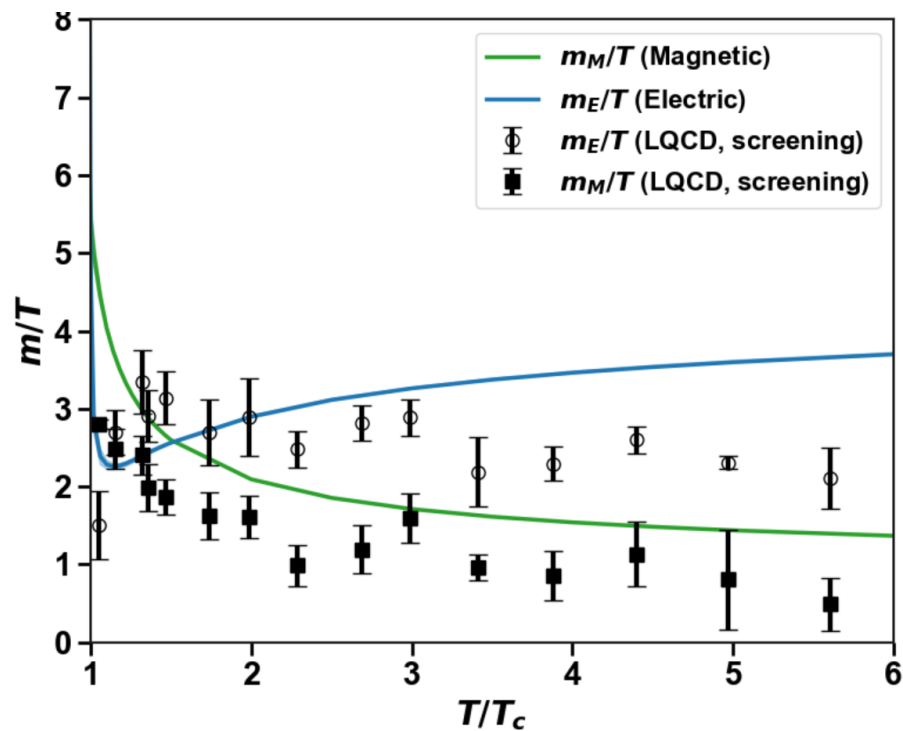
通过神经网络提取色电和色磁胶子质量

训练结果



通过神经网络提取色电和色磁胶子质量

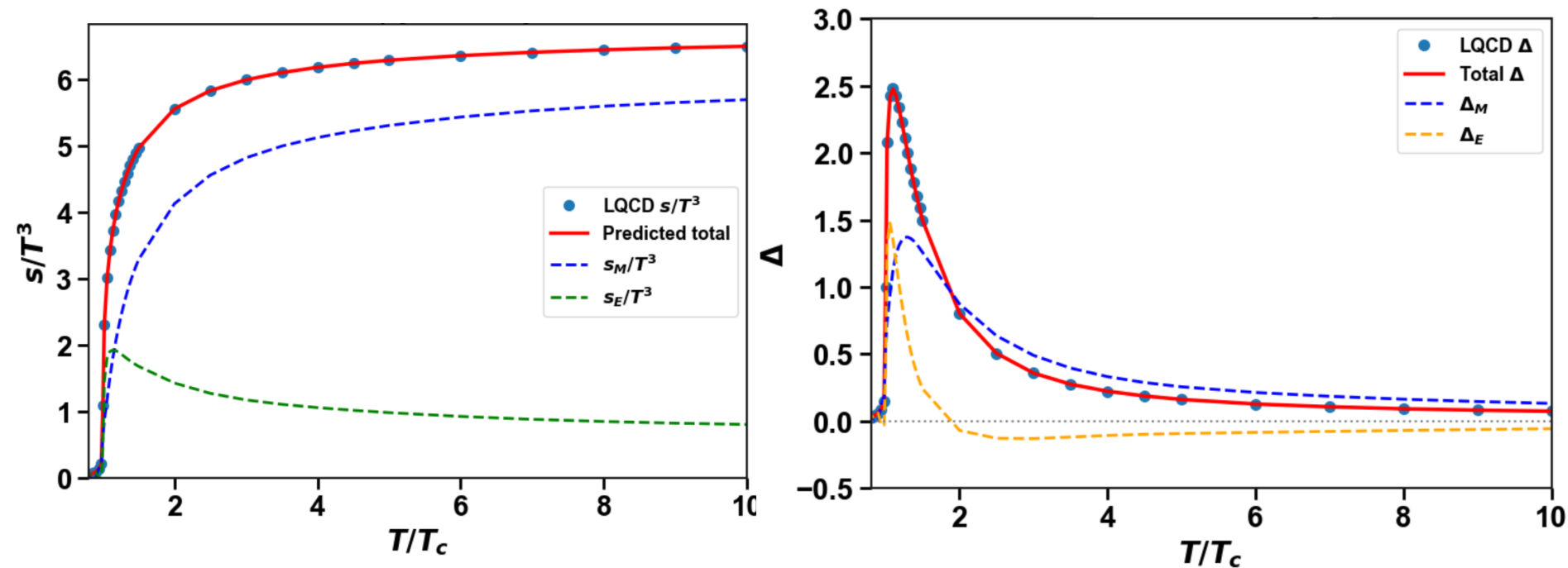
训练结果



20 runs

通过神经网络提取色电和色磁胶子质量

各组分训练结果



色电部分逐渐脱耦

通过神经网络提取色电和色磁胶子质量

色电部分迹反常为负的讨论

迹反常对应**有效自由度**随着外界条件 (T, μ_B) 的变化速率

$$\frac{\langle \Theta \rangle_{T, \mu_B=0}}{T^4} = T \frac{d\nu_T}{dT}, \quad \frac{\langle \Theta \rangle_{T=0, \mu_B}}{\mu_B^4} = \mu_B \frac{d\nu_\mu}{d\mu_B},$$

where we quantify the effective degrees freedom by ν_T
 P/T^4 and $\nu_\mu \equiv P/\mu_B^4$ for hot matter at $\mu_B = 0$ and dense matter at $T = 0$, respectively.

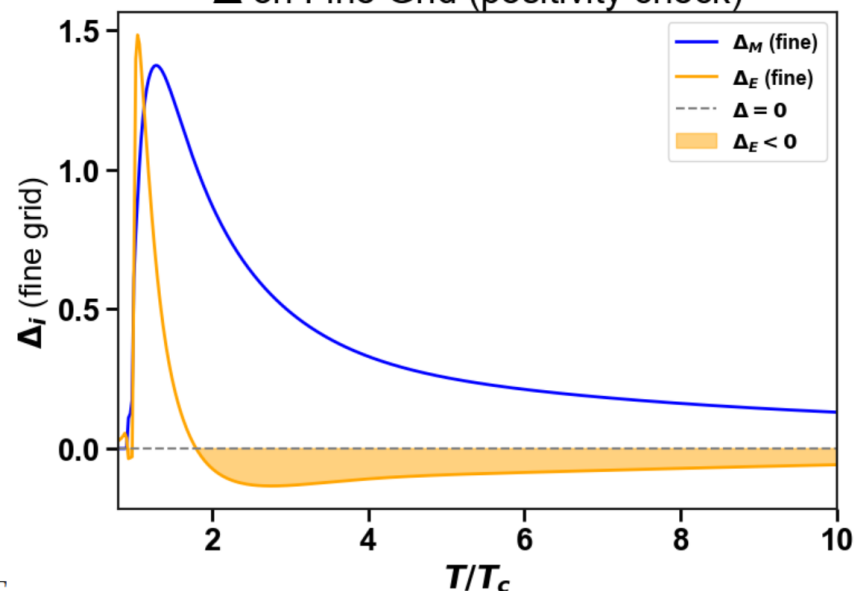
对于胶子系统 $T \uparrow$

对应色电的纵向模式消失

极化模式: $3 \rightarrow 2$

(有质量矢量粒子 $\rightarrow$ 无质量矢量粒子)

Δ on Fine Grid (positivity check)

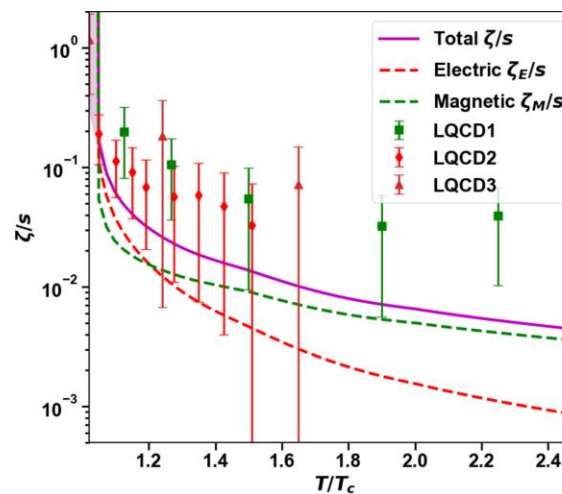
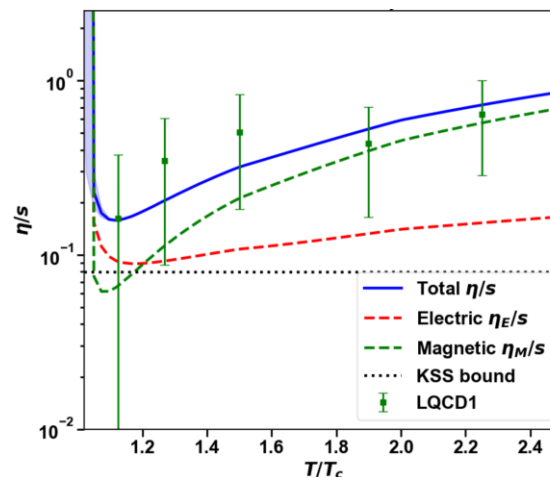
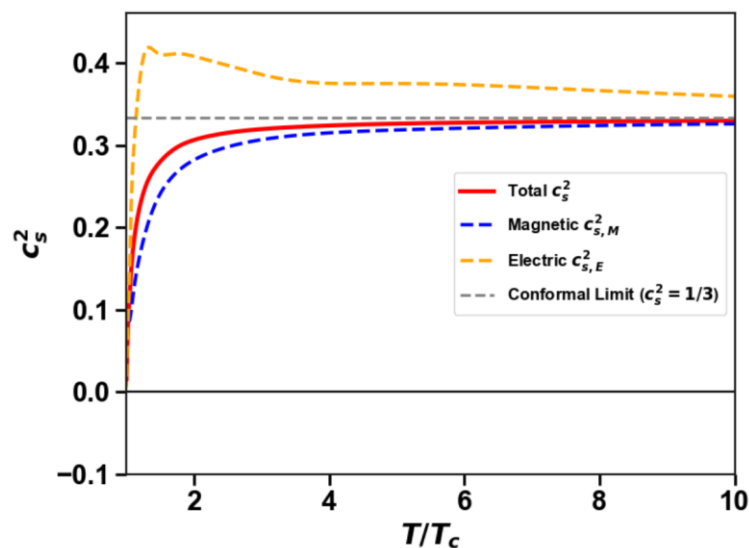


理想气体

$$P = \frac{\pi^2}{90} \frac{k_B^4}{\hbar^3 c^3} g_* T^4$$

通过神经网络提取色电和色磁胶子质量

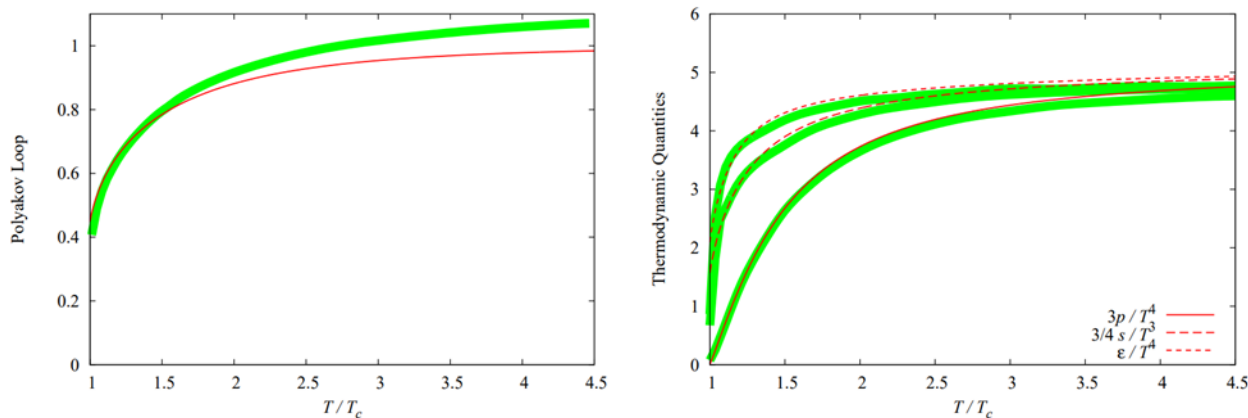
更多数值结果



通过神经网络提取色电和色磁胶子质量

小结

- **数据驱动**：成功利用残差网络结合准粒子模型，提出了一种自下而上的数据驱动方法，直接从格点 QCD 数据中提取色电与色磁胶子的热质量。
- **物理机制揭示**：研究直观地揭示了色电部分在相变过程中的逐渐脱耦现象，并对色电部分迹反常为负的行为（对应纵向模式消失）进行了物理机制上的探讨。验证了当前Polyakov扩展模型可能存在的局限。

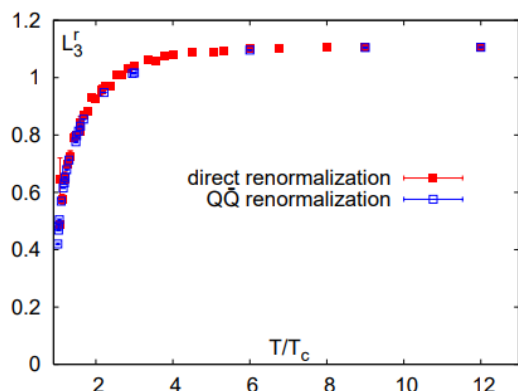


- **流体力学性质验证**：进一步计算了声速以及剪切/体黏滞系数等输运性质，数值结果符合共形极限和理论边界预期。

基于内禀维数的新型退禁闭相变判据

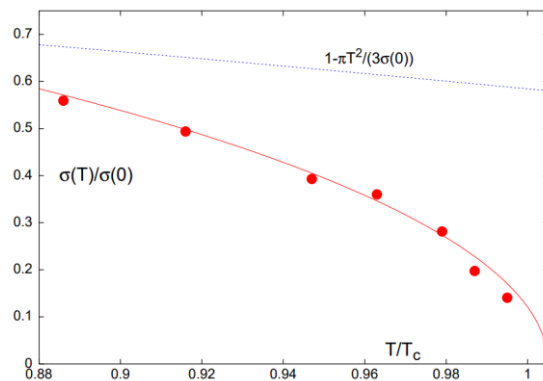
如何定位退禁闭相变?

Polyakov圈



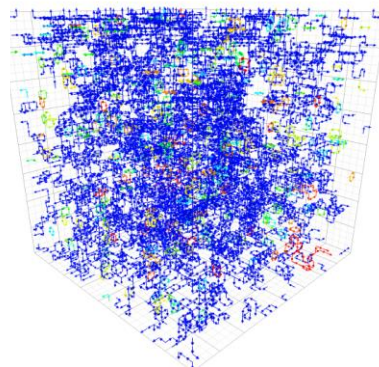
S. Gupta, et. al. (2007)

弦张力

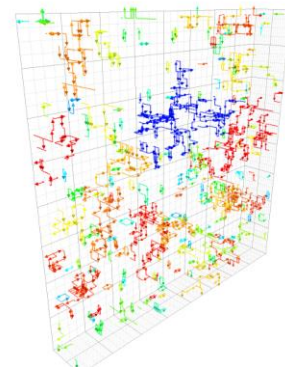


O. Kaczmarek, et. al. (2000)

中心涡旋



J. Mickley, et. al. (2024)

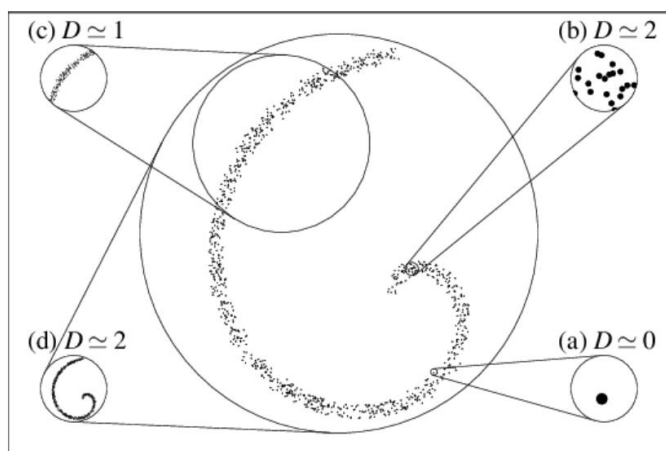


在考虑动力学夸克时不再严格!

基于内禀维数的新型退禁闭相变判据

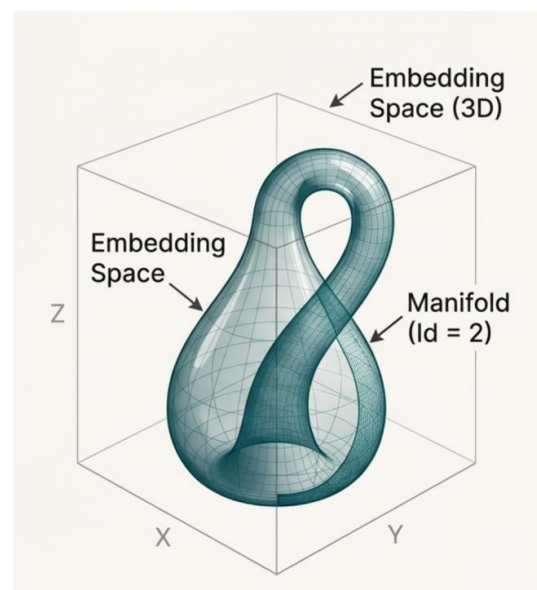
流形中的模式

数据集所处**流形**的**内禀维数(ID)**通常低于数据空间的维度数。



$$\mathbf{x}^i = (x_1^i, x_2^i, \dots, x_N^i)$$

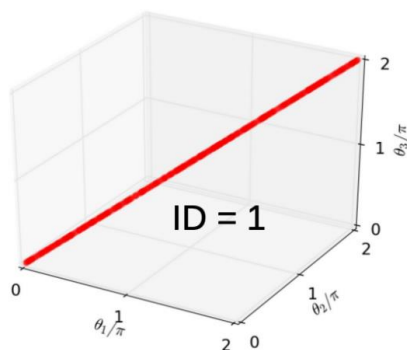
$$\mathbf{x} \sim p(\mathbf{x})$$



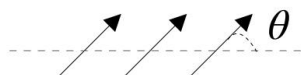
基于内禀维数的新型退禁闭相变判据

示例：L=3的1维XY模型

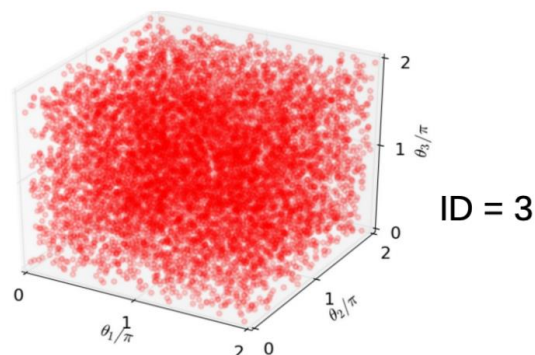
数据集所处**流形**的**内禀维数(ID)**通常低于数据空间的维度数。



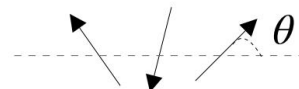
T = 0



$\theta = (\theta_1, \theta_2, \theta_3)$



T = 100

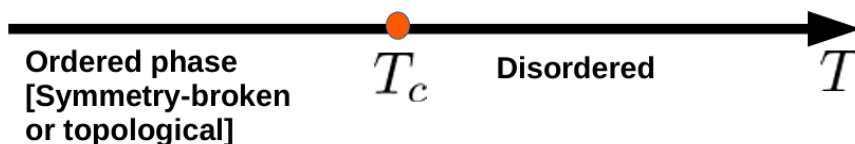


$$H(\theta) = - \sum_{\langle ij \rangle} J \cos(\theta_i - \theta_j)$$

红点：构型数据
坐标轴：各自由度取值

基于内禀维数的新型退禁闭相变判据

研究动机



数据内部的关联
约束ID

数据空间中的相变?

相变附近物理体系的
关联发生突变

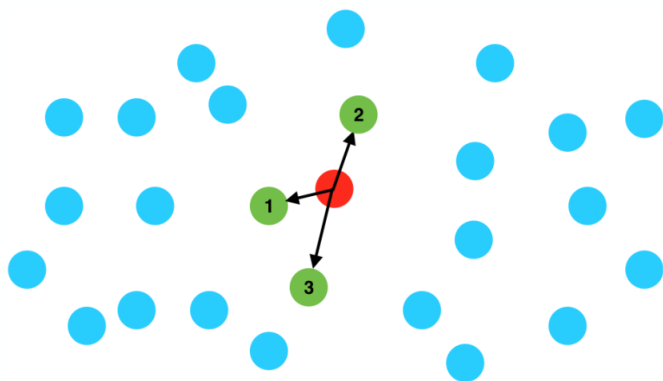
从原始数据中提取系统
信息——普适行为?

基于内禀维数的新型退禁闭相变判据

如何估计ID?

表示学习：类PCA方法、自编码器、变分自编码器等

几何方法：近邻 (nearest-neighbors, NN) 方法



基于NN距离的统计

[如Euclidian, Minkowski距离等]

- 标注数据集中的一点为 i
- 用 r_k 表示点 k 与 i 的距离, 并将其整理为 $[r_0, r_1, \dots, r_k]$
- 其中 $r_0 = 0$, r_1 为最近邻点, r_2 为次近邻点...

基于内禀维数的新型退禁闭相变判据

如何估计ID?

表示学习: 类PCA方法、自编码器、变分自编码器等

几何方法: 近邻 (nearest-neighbors, NN) 方法

Two-NN方法

- 计算数据集 $[1, \dots, N]$ 中每个点 i 的成对距离 (Pairwise distances)
- 对于每个点 i , 找到最短的两个距离 r_1 和 r_2 , 并定义 $\mu \equiv r_2/r_1$
- 将 μ 的值按升序排列, 计算其经验累积分布函数 $F(\mu)$ (Empirical cumulate)
- 对坐标平面上的点集 $\{(\log(\mu_i), -\log(1 - F(\mu_i)))\}$ 进行拟合, 拟合线为一条过原点的直线

[arXiv:1803.06992 \[stat.ML\]](https://arxiv.org/abs/1803.06992)

基于内禀维数的新型退禁闭相变判据

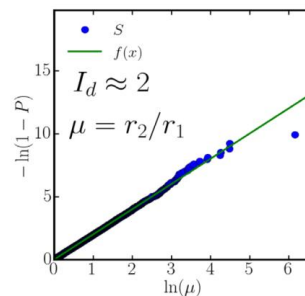
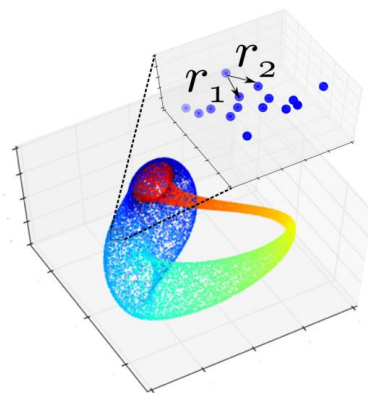
如何估计ID?

表示学习: 类PCA方法、自编码器、变分自编码器等

几何方法: 近邻 (nearest-neighbors, NN) 方法

Two-NN方法

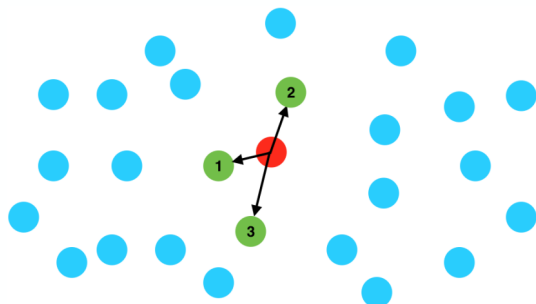
- 计算数据集 $[1, \dots, N]$ 中每个点 i 的 **成对距离** (Pairwise distances)
- 对于每个点 i , 找到最短的两个距离 r_1 和 r_2 , 并定义 $\mu \equiv r_2/r_1$
- 将 μ 的值按升序排列, 计算其**经验累积分布函数** $F(\mu)$ (Empirical cumulate)
- 对坐标平面上的点集 $\{(\log(\mu_i), -\log(1 - F(\mu_i)))\}$ 进行拟合, 拟合线为一条**过原点的直线**



[arXiv:1803.06992](https://arxiv.org/abs/1803.06992) [stat.ML]

技术细节#1

通过two-NN估计ID



- 两个连续近邻点 $l, l-1$ 之间围成的超球壳体积为

$$\Delta v_l = \omega_{I_d} (r_l^{I_d} - r_{l-1}^{I_d}), \omega_{I_d} \text{ 为体积元}$$

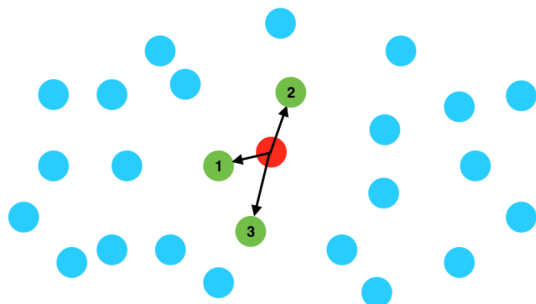
- 可以证明, 若 i 点邻近的密度为常数, 则所有的 Δv_l 都是独立抽取的, 其分布符合:
- $P(\Delta v_l \in [v, v + dv]) = \rho e^{-\rho v} dv$
(齐次泊松过程的球壳体积分布)

假设: 构型在局部自由度 (d.o.f.) 空间中均匀分布

- 流形局部平坦
- 独立同分布 (i.i.d.) 采样构型
- 源自玻尔兹曼分布:
 - $\rho(r) = \rho_0 e^{-\beta(E(r)-E_0)}$, 其中 0 表示在 $r=0$ 处的参考点
 - 在 $r=0$ 附近展开:
$$E(r) \approx E_0 + \nabla E \cdot \vec{r} + \frac{1}{2} \vec{r}^T \mathbf{H} \vec{r} + \dots$$
 - $\rho(r) \approx \rho_i \cdot e^{-\beta(\nabla E \cdot \vec{r} + \dots)}$
在邻域内 $e^{-\beta(\nabla E \cdot \vec{r} + \dots)} \sim 1$
 - $\rho(r)$ 是常数

技术细节#1

通过two-NN估计ID



- 两个连续近邻点 $l, l-1$ 之间围成的超球壳体积为

$$\Delta v_l = \omega_{I_d} (r_l^{I_d} - r_{l-1}^{I_d}), \omega_{I_d} \text{ 为体积元}$$

- 可以证明, 若 i 点邻近的密度为常数, 则所有的 Δv_l 都是独立抽取的, 其分布符合:
- $P(\Delta v_l \in [v, v + dv]) = \rho e^{-\rho v} dv$
(齐次泊松过程的球壳体积分布)

-
- 定义相对差异:

$$R \equiv \frac{\Delta v_i}{\Delta v_j}$$

$$P(R \in [\bar{R}, \bar{R} + d\bar{R}]) = \int_0^\infty dv_i \int_0^\infty dv_j \rho^2 e^{-\rho(v_i + v_j)} \mathbf{1}_{\{\frac{v_i}{v_j} \in [\bar{R}, \bar{R} + d\bar{R}]\}}$$

$$\text{PDF: } g(R) = \frac{1}{(1 + R)^2}$$

- 定义近邻距离的比值:

$$\mu \equiv \frac{r_2}{r_1} \in [1, +\infty)$$

$$R = \mu^{I_d} - 1$$

$$\text{PDF: } f(\mu) = I_d \mu^{-I_d-1}$$

$$\text{CDF: } F(\mu) = (1 - \mu^{I_d})$$

基于内禀维数的新型退禁闭相变判据

二级相变：2维Ising模型与3态Potts模型

$$H_p = -J_p \sum_{(i,j)} \delta(s_i, s_j)$$

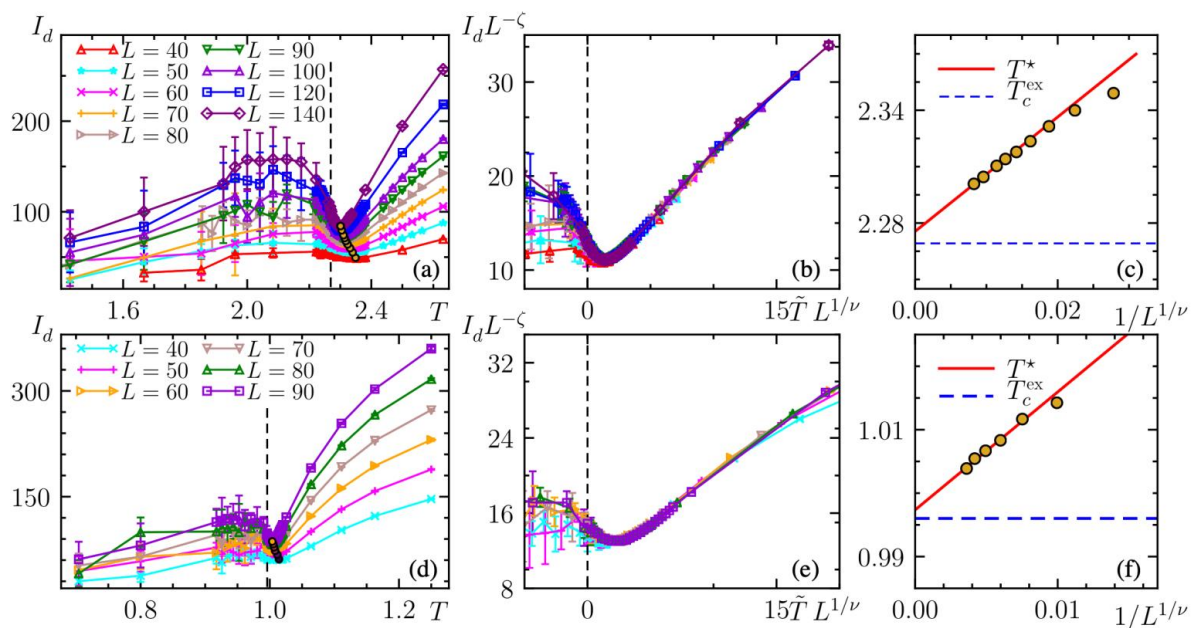


FIG. 2. Second-order phase transition. (a)–(c) Ising model. (d)–(f) $q = 3$ Potts model. (a,d) I_d as a function of T . Error bars are standard deviations associated with a distribution of n realizations of I_d (we typically consider $n \geq 5$). (b,e) Data collapse of I_d based on the finite-size scaling discussed in the main text. The best data collapse of the results gives $T_c = 2.283(2)$, $\nu = 1.02(2)$, and $\zeta = 0.410(5)$ for the case of the Ising model, and $T_c = 0.996(2)$, $\nu = 0.805(5)$, and $\zeta = 0.420(2)$ for the case of the Potts model. (c,f) finite-size scaling of the minimum temperature T^* (see text); the horizontal line is the exact result for T_c . The extrapolation returns $T_c = 2.2784(2)$ and $T_c = 0.9970(3)$ for the Ising and Potts cases, respectively.

T.M. Santos, X. Turkeshi, M. Dalmonte, A. Rodriguez, PRX 11, 011040 (2021)

$N = 5 \times 10^4$

技术细节#2

临界指数

有限尺寸标度 (FSS) 理论

$$I_d = L^\zeta f(\xi/L)$$

$$\xi = (T - T_c)^{-\nu}$$

关联长度

ν is a critical exponent, ζ a scaling exponent associated with the divergence of I_d at T_c

近邻距离的分布取决于体系的多
体关联

关联增强会将数据挤压到一个
更加简单的流形中，从而
降低ID

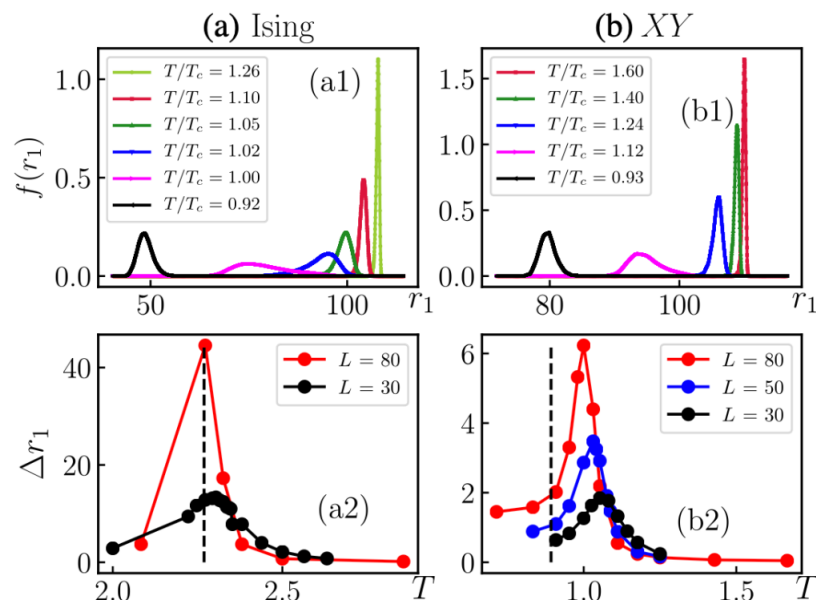
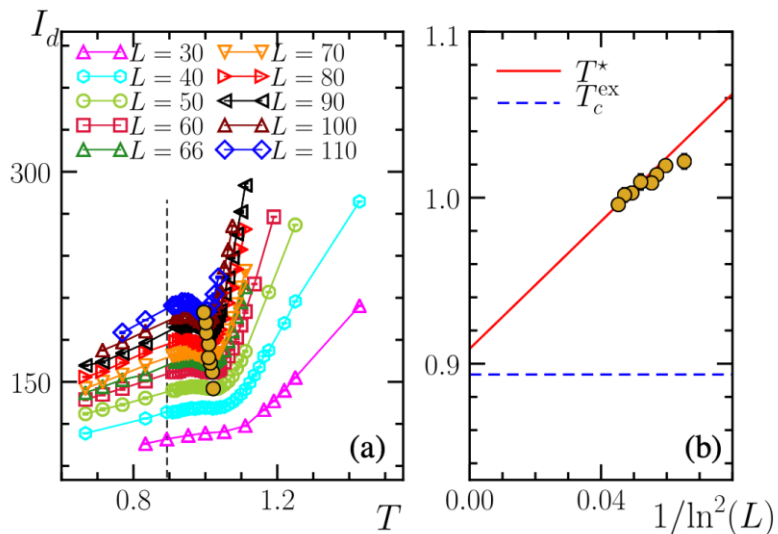


FIG. 6. Statistics of first nearest-neighbor distances, r_1 . In panels (a1) and (b1), we show the kernel density estimation of the probability density function of r_1 for the Ising and XY data sets, respectively. All the results have $L = 80$. Panels (b1) and (b2) show the temperature dependence of the variance associated with the distribution functions from panel (a) for different system sizes. Results for the second nearest-neighbor distances, r_2 , are qualitatively the same.

T.M. Santos, X. Turkeshi, M. Dalmonte, A. Rodriguez, PRX 11, 011040 (2021)

BKT相变&一级相变

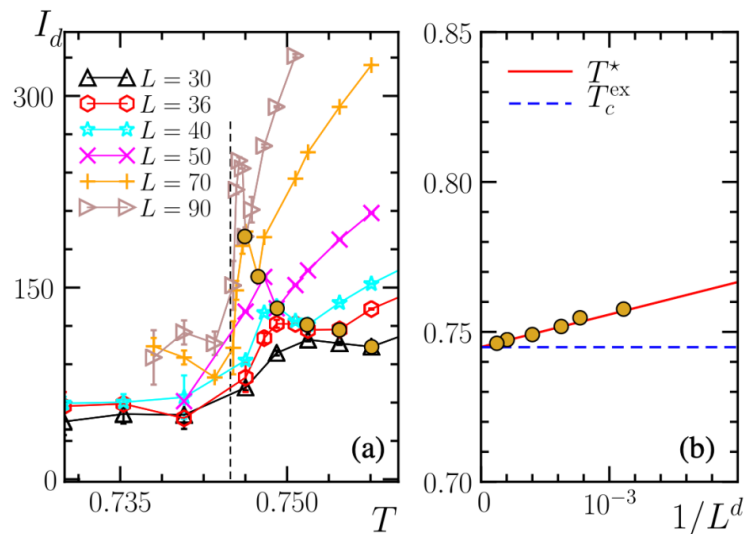
2维XY模型



$$I_d = L^\zeta f(\xi/L)$$

$$\xi = \exp(a/\sqrt{T - T_c})$$

Potts模型 (q=8)



$$I_d = L^\zeta f(\xi/L)$$

$$\xi_8 = 23.9$$

correlation length

$$T_c(L) - T_c \sim \frac{1}{L^d}$$

$$N = 5 \times 10^4$$

T.M. Santos, X. Turkeshi, M. Dalmonte, A. Rodriguez, PRX 11, 011040 (2021)

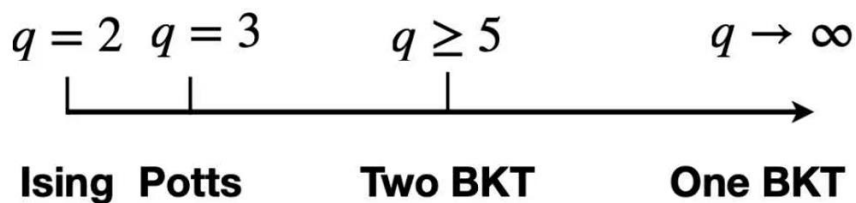
基于内禀维数的新型退禁闭相变判据

Why ID?

Feature	Correlation Length (ξ)	Intrinsic Dimension (Id)
Prerequisites	Requires knowing the Order Parameter	None (Unsupervised)
Topological Phases	Often fails (requires non-local operators)	Works (Detects manifold topology)
Calculation	Expensive (Fit decay of $C(r)$)	Cheap (Nearest-neighbor statistics)
Generality	Specific to the model	Universal across models

多相变体系

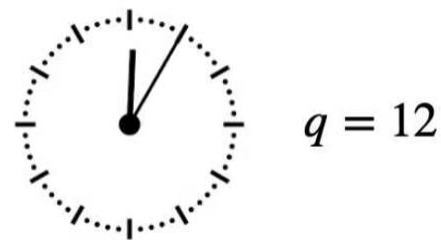
2维q态Clock模型



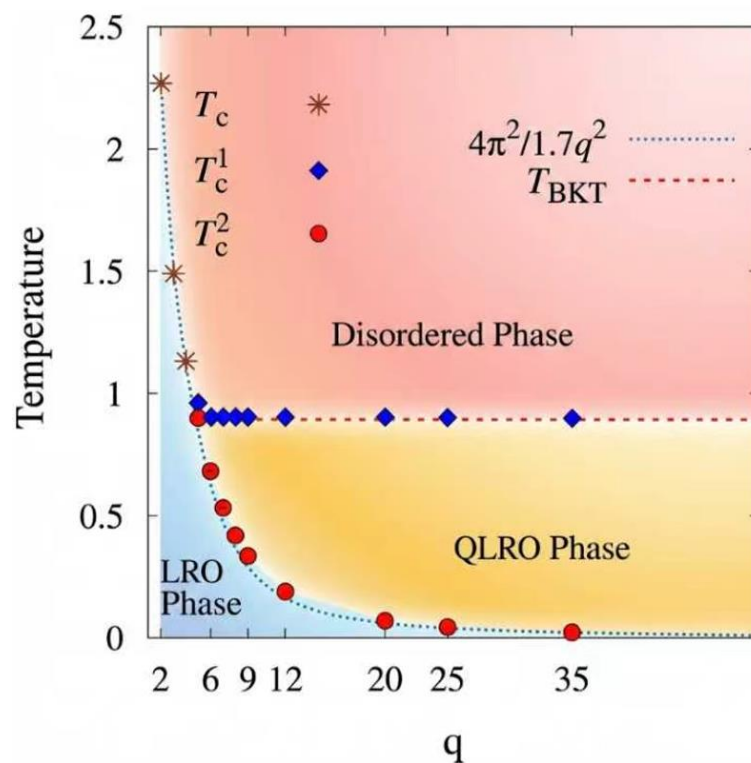
$$H(\theta) = - \sum_{\langle ij \rangle} J \cos(\theta_i - \theta_j)$$

$$\theta_s = \frac{2\pi s}{q} \quad s = 0, 1, \dots, q-1$$

离散化版本的XY模型

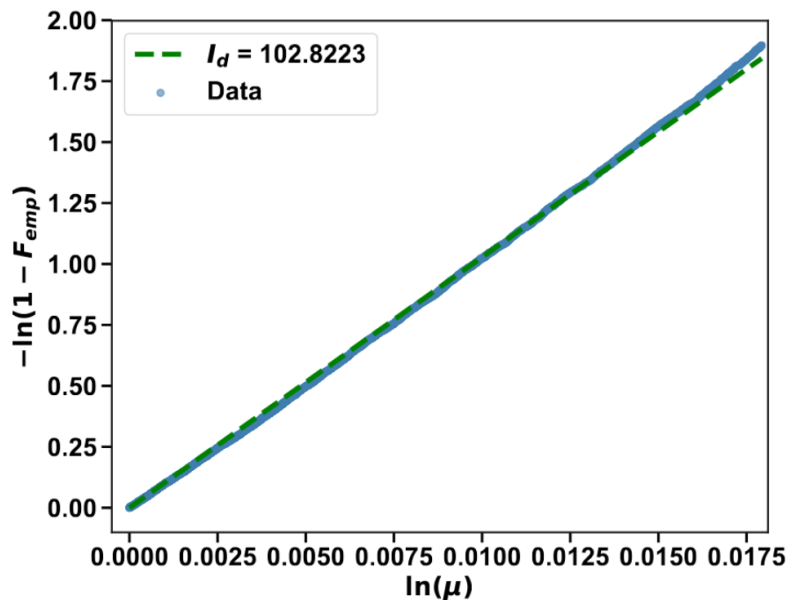


Phys. Rev. E 98, 032109 (2018)

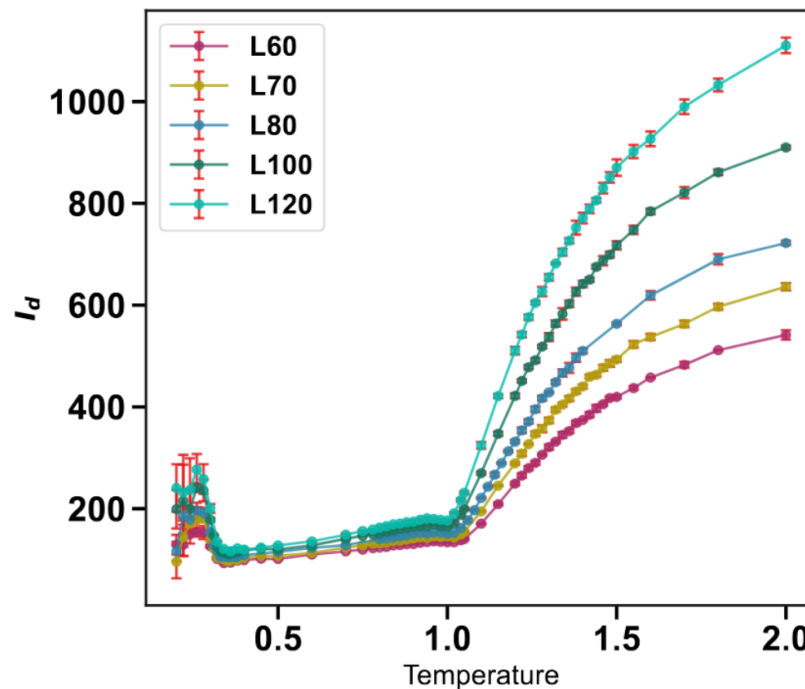


基于内禀维数的新型退禁闭相变判据

2维q态Clock模型 ($q=9$)



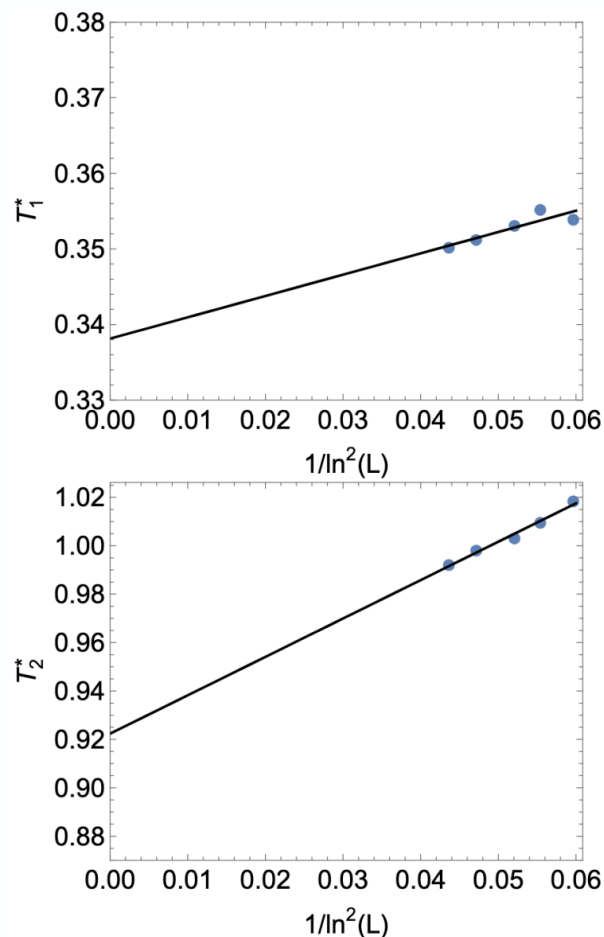
$$T = 0.5, L = 60, N = 10^4$$



- 中间相出现平台行为 (准长程序)
- 在不同相中ID近似线性增长

基于内禀维数的新型退禁闭相变判据

2维q态Clock模型 (q=9)



有限尺寸标度 (FSS) 理论

$$I_d = L^\zeta f(\xi/L)$$

$$\xi = \exp(a/\sqrt{T - T_c})$$

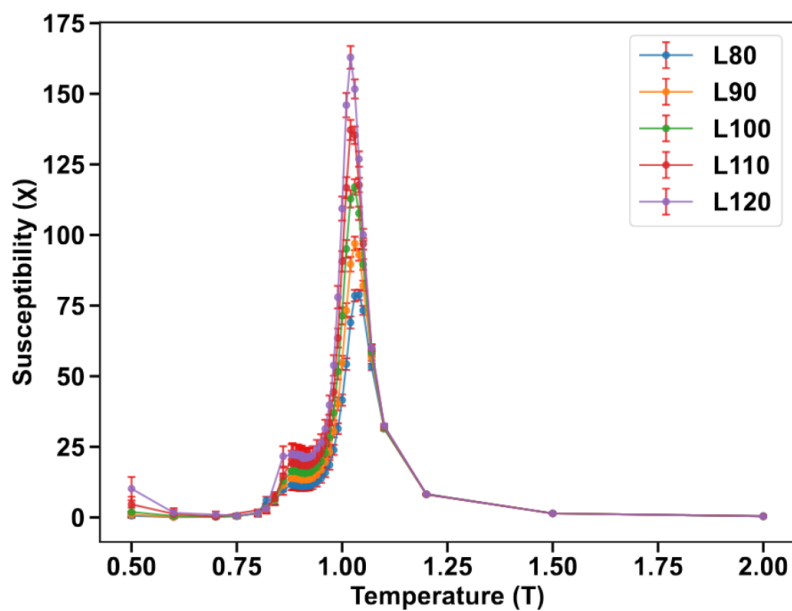
关联长度

ν is a critical exponent, ζ a scaling exponent associated with the divergence of I_d at T_c

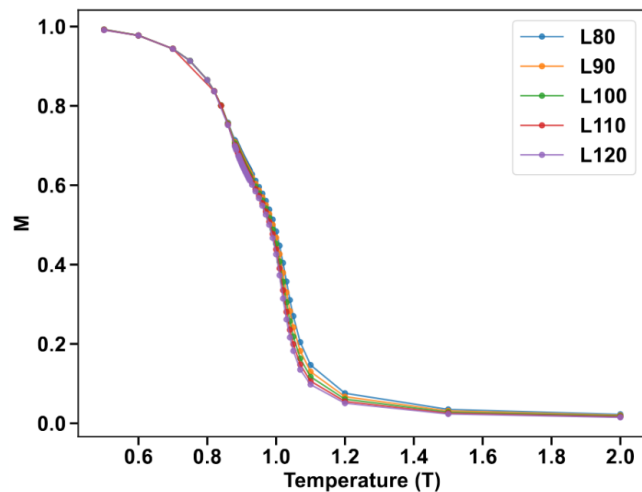
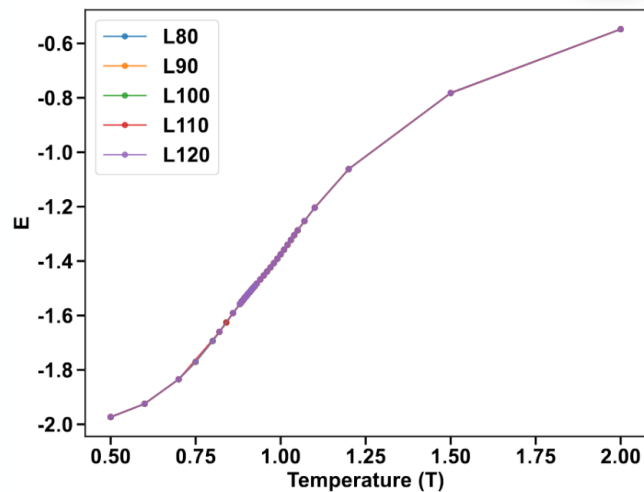
$$T_1 \sim 0.338, T_2 \sim 0.924$$

基于内禀维数的新型退禁闭相变判据

2维q态Clock模型 ($q=5$)

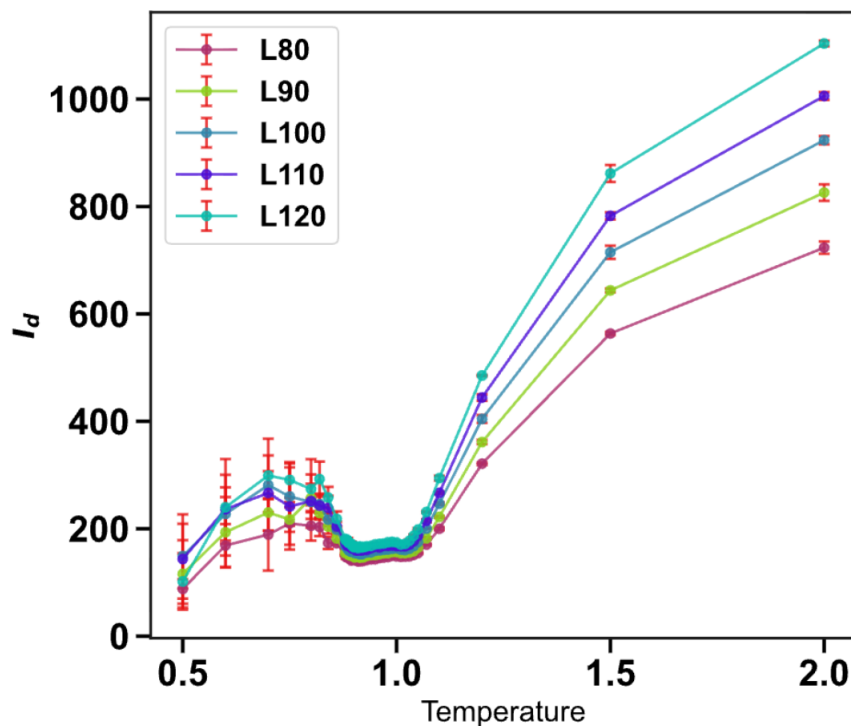


$N = 10^4$

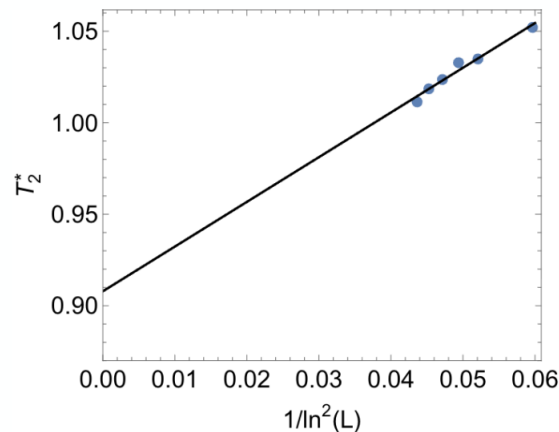
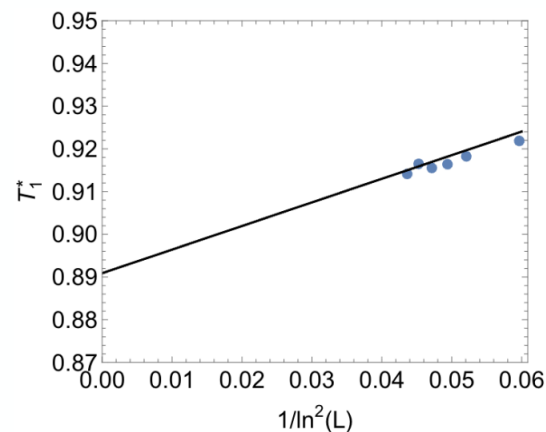


基于内禀维数的新型退禁闭相变判据

2维q态Clock模型 ($q=5$)



$N = 10^4$



$T_1 \sim 0.891, T_2 \sim 0.910$

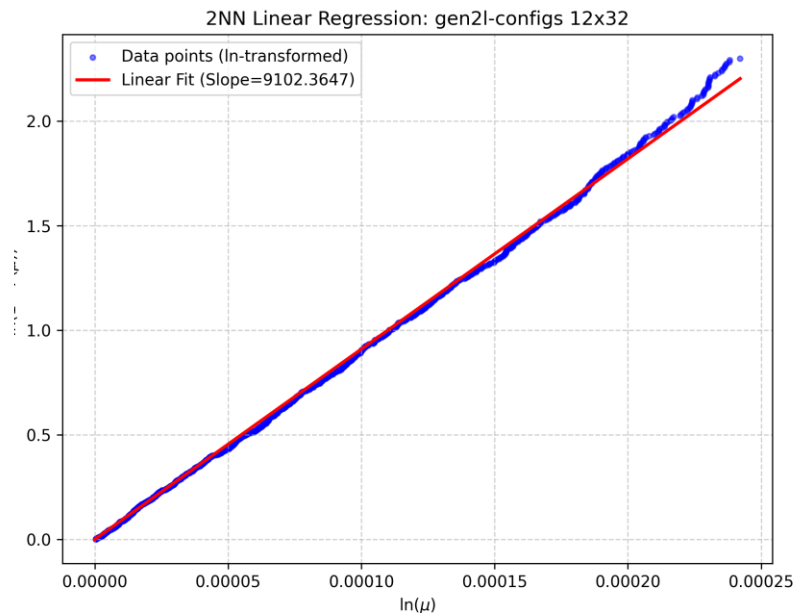
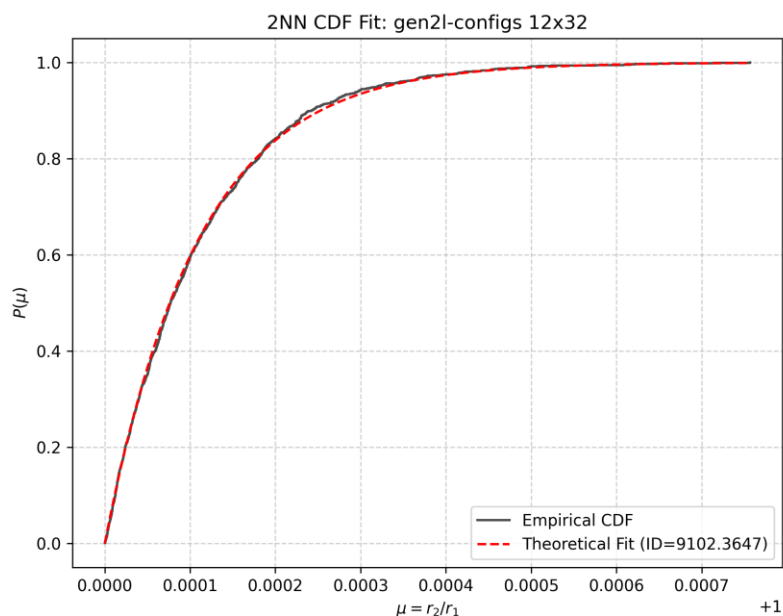
基于内禀维数的新型退禁闭相变判据

格点QCD数据 (in collaboration with FASTSUM group)

TABLE I. FASTSUM Generation 2L ensembles used in this work. The lattice size is $32^3 \times N_\tau$, with temperature $T = 1/(a_\tau N_\tau)$. The spatial lattice spacing is $a_s = 0.11208(31)$ fm with renormalised anisotropy $\xi = a_s/a_\tau = 3.453(6)$, and the pion mass is $m_\pi = 239(1)$ MeV [38]. The estimate for T_c comes from an analysis of the renormalised chiral condensate, which provides $T_c = 167(3)$ MeV [13, 39]. Full details of these ensembles may be found in Refs. [13, 39].

N_τ	128	64	56	48	40	36	32	28	24	20	16	12	8
T (MeV)	47	95	109	127	152	169	190	217	253	304	380	507	760
T/T_c	0.284	0.569	0.650	0.758	0.910	1.01	1.14	1.30	1.52	1.82	2.28	3.03	4.55

$N = 1000$



基于内禀维数的新型退禁闭相变判据

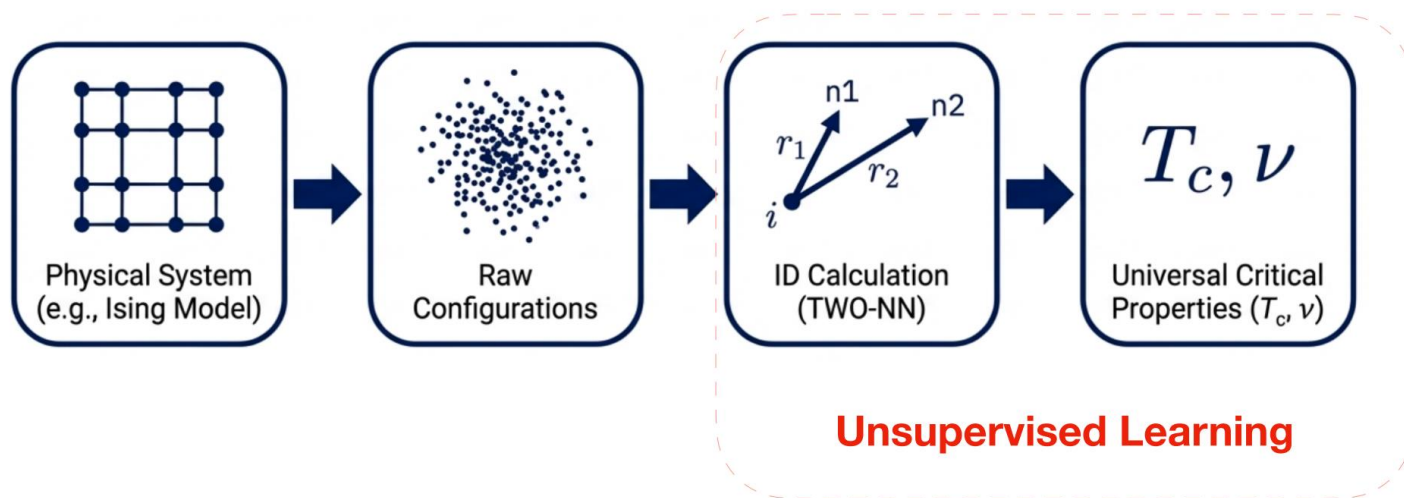
格点QCD数据 (in collaboration with FASTSUM group)

可能存在的问题

- ~~维度灾难：构型空间维度过高&数据点太少~~
- 格点数据的温度点过于稀疏导致可能错过临界点
- 温度随虚时格数变化带来额外自由度

基于内禀维数的新型退禁闭相变判据

Pipeline



配置/构型的选择并不局限于格点配置！

- 格点场配置
- 大语言模型（LLM）生成的文本 [[arXiv:2405.17088](#), [arXiv:2501.16241](#)]
- 神经网络参数 [[B. Yasaman, et. Al. \(2020\)](#)]
- 蛋白质序列 [[arXiv:1902.05158](#)]
- ...

基于内禀维数的新型退禁闭相变判据

小结

- **无监督的几何拓扑判据**：提出了一种无需预先知晓序参量的全新相变定位判据，通过挖掘数据集所处流形的内禀维数 (ID) 变化，即可捕捉系统关联的物理突变。
- **普适性与鲁棒性验证**：利用 Two-NN 方法有效估算 ID，在二维 Ising、Potts、XY 及 Clock 等多种经典模型中均取得成功，精准识别了二级相变、一级相变及 BKT 相变，且完美契合有限尺寸标度理论。
- **广泛的应用前景**：该数据驱动的非监督学习路径不仅适用于物理格点场配置，还展现出向大语言模型 (LLM) 文本、神经网络参数以及蛋白质序列等复杂系统推广的巨大潜力