Complex control variates

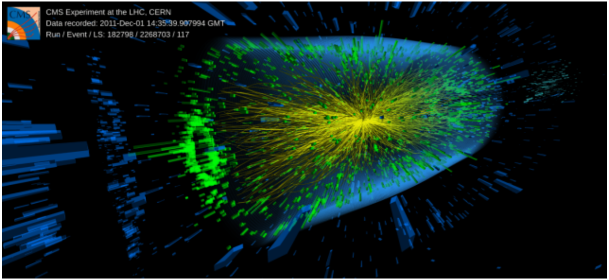
Yukari Yamauchi

- arXiv:2205.12303 [hep-lat] with Scott Lawrence and Hyunwoo Oh
- arXiv:2212.14606 [hep-lat] with Scott Lawrence
- arXiv:2311.13002 [hep-lat] with Scott Lawrence

November 24th, 2023, Large-scale lattice QCD simulation and application of machine learning, university of Tsukuba

INSTITUTE for NUCLEAR THEORY

Sign problems in lattice QCD



Tom McCauley/CMS/CERN

Path integral

$$\langle \mathcal{O}(t_0) \rangle = \mathrm{Tr}\left[e^{-\beta H}\, e^{iHt_0}\, \mathcal{O}\, e^{-iHt_0} \right] = \frac{1}{Z} \int \mathcal{D}[\psi, U]\, e^{-S_{\mathrm{SK}}}\, \mathcal{O}(t_0)$$

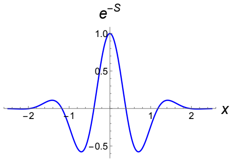
The average phase

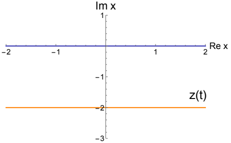
$$\langle \sigma \rangle = \frac{\int \mathcal{D}[\psi, U]\, e^{-S_{\mathrm{SK}}}}{\int \mathcal{D}[\psi, U]\, |e^{-S_{\mathrm{SK}}}|} \propto e^{-V}$$

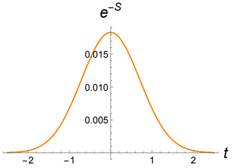
Methods

1. Contour deformation / complex normalizing flow

Example: $S(x) = x^2 - 4ix$







Demonstration: scalar fields theories in $0+1$ and $1+1$-d

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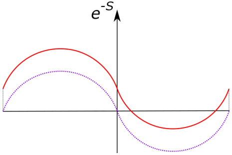
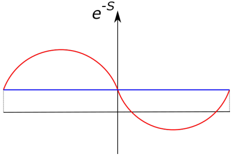
2. Complex control variates (subtraction)



$\rightarrow$



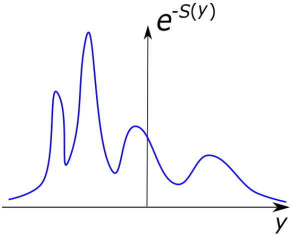
Demonstration: Spin system, Thirring model in $1+1$-d

Normalizing flows — when no sign problem

Normalizing flow[1] $\vec{y} = f(\vec{x})$:

$$\det\left(\frac{\partial \vec{y}}{\partial \vec{x}}\right) e^{-S(\vec{y})} = \mathcal{N} \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi}} e^{-x_i^2/2} = \mathcal{N} G_N(\vec{x})$$

Some distribution

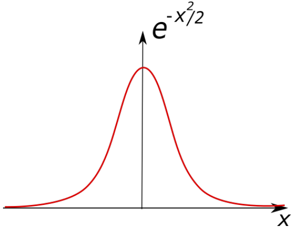


Map

$\leftrightarrow$

$y(x)$

Simple Gaussian distribution



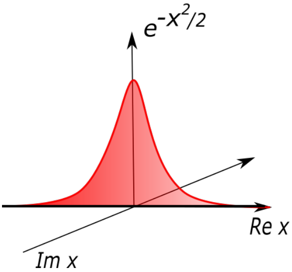
if such a map exists, then

$$\langle \mathcal{O} \rangle = \frac{\int_{\mathbb{R}^N} \mathcal{D}\vec{y}\ e^{-S(\vec{y})} \mathcal{O}(\vec{y})}{\int_{\mathbb{R}^N} \mathcal{D}\vec{y}\ e^{-S(\vec{y})}} = \frac{\int_{\mathbb{R}^N} d\vec{x}\ G_N(\vec{x}) \mathcal{O}(\vec{y}(\vec{x}))}{\int_{\mathbb{R}^N} d\vec{x}\ G_N(\vec{x})}$$

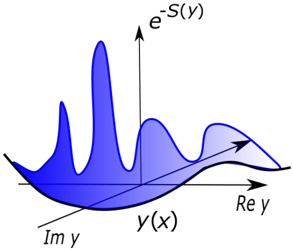
[1] M. Albergo et al. Phys. Rev. D 100, 034515(2019)
K. A. Nicoli, et al. Phys. Rev. E 101, 023304(2020)

Complex normalizing flow[2]/contour deformations

$$\mathcal{N} G_N(\vec{x}) = \det\left(\frac{\partial \vec{y}}{\partial \vec{x}}\right)\ e^{-S(\vec{y}(\vec{x}))}$$



Map
$\leftrightarrow$
$y(x)$



Expectation values:

$$\frac{\int_{\mathbb{R}^N} d\vec{x}\ G_N(\vec{x})\mathcal{O}(y(x))}{\int_{\mathbb{R}^N} d\vec{x}\ G_N(\vec{x})} = \frac{\int_{\vec{y}(\mathbb{R}^N)} d\vec{y}\ e^{-S(\vec{y})}\mathcal{O}(\vec{y})}{\int_{\vec{y}(\mathbb{R}^N)} d\vec{y}\ e^{-S(\vec{y})}} \stackrel{?}{=} \langle \mathcal{O} \rangle$$

Perfect complex normalizing flow $\rightarrow$ No sign problems!

[2] S. Lawrence and YY, arXiv:2101.05755 [hep-lat]

Machine-learn a map

Contour deformation

Loss function: $L = -\log\langle\sigma\rangle$

The gradient of $\langle\sigma\rangle$ is **sign-free**[3]!

$$\partial_v(-\log\langle\sigma\rangle) = -\frac{\int_{\mathcal{C}} \mathcal{D}\phi\, (\partial_v \operatorname{Re} S)\left|e^{-S}\right|}{\int_{\mathcal{C}} \mathcal{D}\phi\, \left|e^{-S}\right|}$$

- Needs MCMC sampling
- Can find "good enough" contours

Complex normalizing flow

Loss function:

$$L = \left\langle \left| \det\left(\frac{\partial y(x_i)}{\partial x_i}\right) e^{-S(y(x_i))} - \mathcal{N}\, G_N(x_i) \right| \right\rangle_{G_N}$$

- No MCMC sampling
- Find only very good contours

[3]A. Alexandru, P. Bedaque, H. Lamm, and S. Lawrence, arXiv:1804.00697 [hep-lat]

Normalizing flows for complex coupling model in $0+1$-d[4]

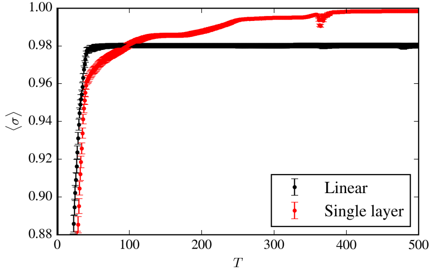
$$S=\sum_{i=1}^{N}\frac{m}{2}\phi_i^2+\frac{(\phi_i-\phi_{i-1})^2}{2}+\lambda\phi_i^4,\ \text{with}\ \lambda\in\mathbb{C}$$

Neural network $\vec{\phi}(\vec{x})=f(\vec{x})+ig(\vec{x})$, σ =sigmoid

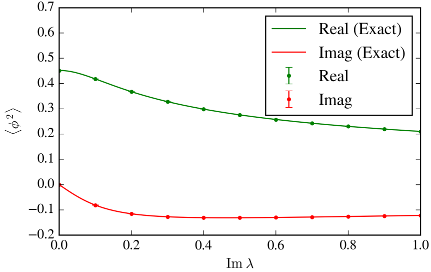
$$f,g(\vec{x})=\left(L_{N,N}+L_{N,2N}\otimes\sigma\otimes L_{2N,2N}\cdots L_{2N,2N}\otimes\sigma\otimes L_{2N,N}\right)\vec{x}$$

Demonstration: $N=10, m=0.5$

$\lambda=0.1+i$



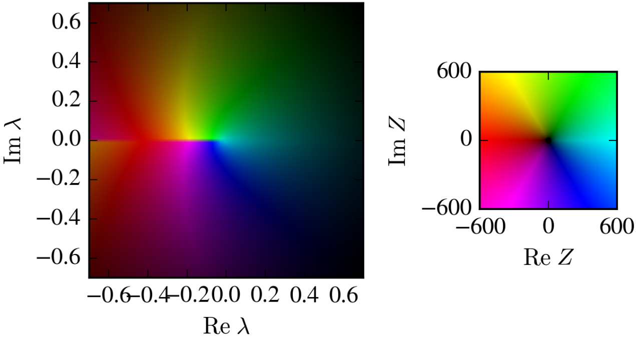
$\mathrm{Re}\,\lambda=0.1$



[4] S. Lawrence, H. Oh, and YY, arXiv:2205.12303 [hep-lat]

Partition function in $0 + 1$-dimensions

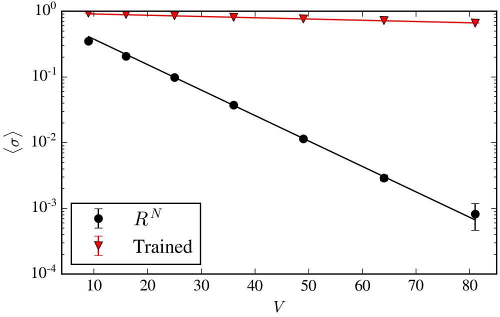
$$S = \sum_{i=1}^{N} \frac{m}{2}\phi_i^2 + \frac{(\phi_i - \phi_{i-1})^2}{2} + \lambda\phi_i^4, \text{ with } \lambda \in \mathbb{C}$$



- $N = 10$, $m = 0.5$
- 1 internal layer
- Adiabatic training

Contour deformation for complex coupling model in $1+1$-d

The average sign over the lattice size V



- $m = 0.5, \lambda = i$
- linear contour $\tilde{\phi}(\phi) = \phi + M_R\phi + iM_I\phi$
- square lattice

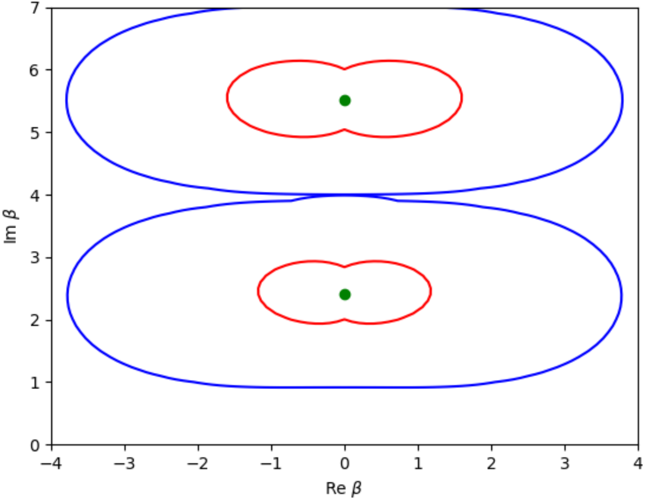
Question of existence

Do complex normalizing flows exist for any lattice field theories?

NO

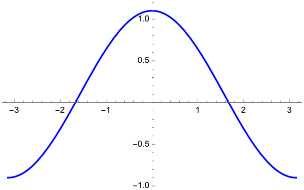
(Non)-existence in $U(1)$ gauge theory in $1+1$-d

$$e^{-S} = \prod_i e^{\beta \cos(\theta_i)}$$



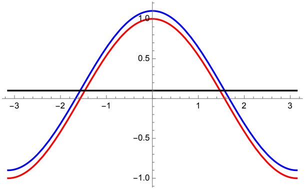
Complex control variates

$\mathcal{O} = \cos\theta + \epsilon$



$\rightarrow$

$\mathcal{O} - f = \epsilon$



The idea is very simple...

Subtract a function f from $\mathcal{O}$!!

Without changing physics, so

$$\langle \mathcal{O} \rangle = \langle \mathcal{O} - f \rangle \;\; \text{but} \;\; \mathrm{Var}(\mathcal{O}) > \mathrm{Var}(\mathcal{O} - f)$$

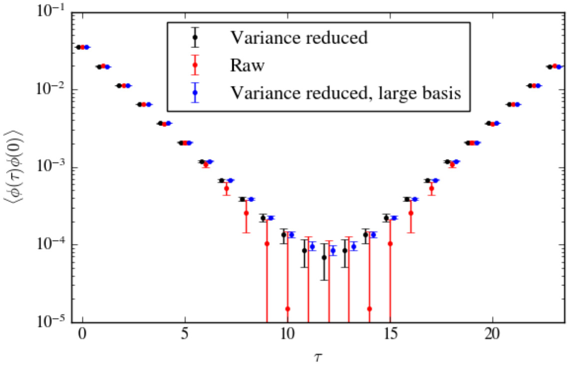
So we strictly impose

$$\langle f \rangle = \int \mathcal{D}[\phi] \, e^{-S(\phi)} \, f(\phi) = 0$$

Variance reduction for signal-to-noise problem[5]

Lattice scalar ϕ^4 theory in Euclidean

$$S = \sum_{\langle r,r'\rangle} \frac{(\phi(r)-\phi(r'))^2}{2} + \sum_r \left[\frac{m^2}{2}\phi^2(r) + \frac{\lambda}{24}\phi^4(r)\right]$$



24×24 lattice, $m^2 = 0.0, \lambda = 2.0$

[5]T. Bhattacharya, S. Lawrence, and J. Yoo, arXiv:2307.14950 [hep-lat]

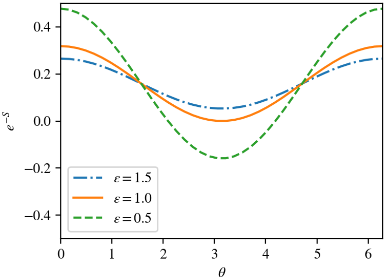
Existence of control variates

Perfect control variates always exist!

Example:

$$e^{-S(\theta;\epsilon)} = \cos(\theta) + \epsilon, \quad \theta \in [0, 2\pi)$$

What is the perfect control variates?



More generally, for any e^{-S}

$$f(x) = e^{-S(x)} - \frac{\int \mathcal{D}x \; e^{-S(x)}}{\int \mathcal{D}x \; 1}$$

(Perfect control variates are not unique)

Notes on control variates

Other strength of control variates

- Include all contour deformation methods
- No Jacobian
- Can be applied to discrete field space

How do we find good control variates?

1. Analytical (perturbative) approaches
   - S. Lawrence, arXiv:2009.10901[hep-lat]
   - S. Lawrence and **YY**, arXiv:2212.14606 [hep-lat]

2. Numerical approaches
   - Start with ansatz and optimize
   - Machine learning

Demonstration: Classical Ising model, Thirring model in $1+1$-d

Demonstration: Classical Ising model (Lee-Yang zeros)

Classical Ising model: $S(\vec{s}) = -J\sum_{\langle i,j\rangle} s_i s_j - h\sum_i s_i$

Lee-Yang Theorem: the partition function is **0** only on with imaginary h.

Goal: Compute $Z = \sum_s e^{-S}$ at **purely imaginary magnetic field**

Measure

$$\frac{Z(h)}{Z(h{=}0)} = \frac{\sum_s \exp\Big(J\sum_{\langle i,j\rangle} s_i s_j\Big)\ \exp\big(h\sum_i s_i\big)}{\sum_s \exp\Big(J\sum_{\langle i,j\rangle} s_i s_j\Big)} = \left\langle e^{h\sum_i s_i}\right\rangle_Q$$

By replacing

$$e^{h\sum_i s_i} \to e^{h\sum_i s_i} - \mathbf{CV}$$

and optimize **CV** to minimize

$$\mathrm{Var}\left(e^{h\sum_i s_i} - \mathbf{CV}\right)$$

Extreme learning machine

1. Prepare basis functions

$$\left\{\sum s, \cos(\sum s), \sin(\sum s)\right\} \times s \times S(h=0)^n$$

$(0 \le n \le 3)$

2. Input basis functions to ELM
3. Take "divergence"

$$F_i = f(s_i) - f(-s_i)$$

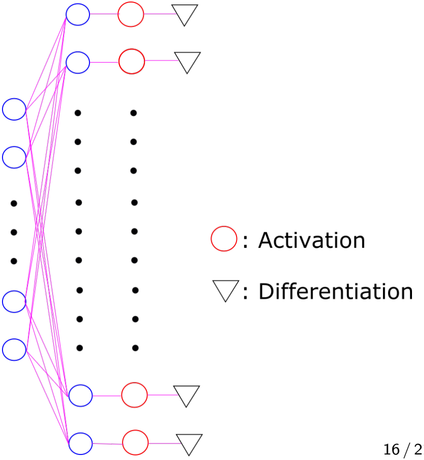
4. The $CV = \sum_i c_i F_i$

The coefficients c_i are optimized by estimating

$$M_{ij} = \langle F_i F_j \rangle, v_j = \langle \mathcal{O} F_i \rangle$$

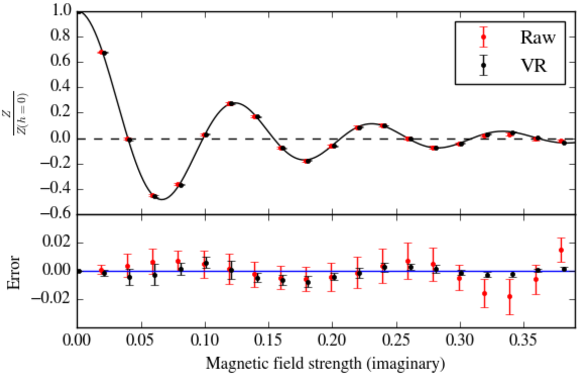
and

$$c = M^{-1}\ v$$



Classical Ising model[6]

At purely imaginary h, $J = 0.4 < J_c \approx 0.441$, 8×8 lattice:



- Raw: 5k samples for Z
- VR: 5k samples to optimize, 5k samples for Z

[6] S. Lawrence and **YY**, in preparation

Measurement of observables

Idea 1. No subtraction in the numerator

$$\langle \mathcal{O} \rangle = \frac{\int \mathcal{D}x \; e^{-S(x)} \mathcal{O}}{\int \mathcal{D}x \; e^{-S(x)}} = \frac{\int \mathcal{D}x \; (e^{-S(x)} - f(x)) \frac{e^{-S(x)}}{e^{-S(x)} - f(x)} \mathcal{O}}{\int \mathcal{D}x \; e^{-S(x)} - f(x)}$$

(Phase fluctuation moved from denominator to numerator.)

Idea 2. Subtract $\nabla \cdot (\mathcal{O}\vec{v})$ anyway

$$\langle \mathcal{O} \rangle = \frac{\int \mathcal{D}x \; e^{-S(x)} \mathcal{O} - \nabla \cdot (\mathcal{O}\vec{v})}{\int \mathcal{D}x \; e^{-S(x)} - \nabla \cdot \vec{v}}$$

$$= \frac{\int \mathcal{D}x \; (e^{-S(x)} - \nabla \cdot \vec{v}) \left(\mathcal{O} + \frac{\vec{v} \cdot \nabla \mathcal{O}}{e^{-S(x)} - \nabla \cdot \vec{v}} \right)}{\int \mathcal{D}x \; e^{-S(x)} - \nabla \cdot \vec{v}}$$

Hoping that the "extra term" won't cause signal-noise problem.

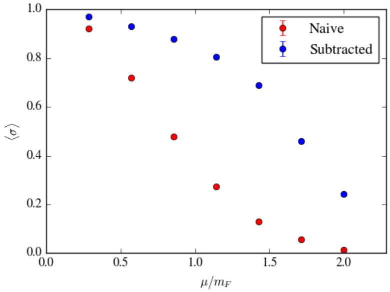
This seems to work for the density operator.... (why?)

Thirring model in 1 + 1-dimension

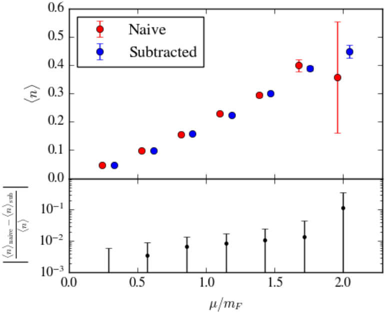
$$S = \sum_{x,\nu} \frac{2}{g^2} (1 - \cos A_\nu(x)) - \log\det K, A_\nu \in [0, 2\pi)$$

with the Dirac matrix ($\eta_0 = (-1)^{\delta_{0,x_0}}$ and $\eta_1 = (-1)^{x_0}$)

$$K[A]_{xy} = m\delta_{xy} + \frac{1}{2}\sum_{\nu=0,1} \eta_\nu e^{iA_\nu(x)+\mu\delta_{\nu,0}}\delta_{x+\nu,y} - \eta_\nu e^{-iA_\nu(y)-\mu\delta_{\nu,0}}\delta_{y+\nu,x}$$



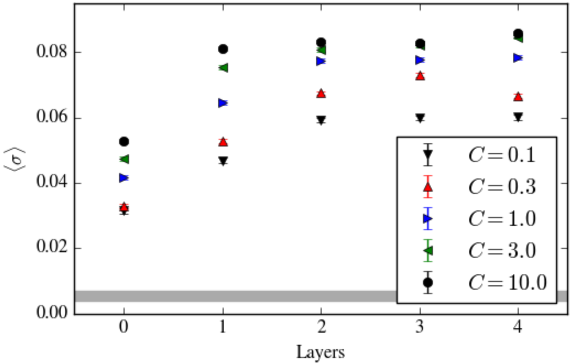
Average sign



Density

- 4×4 lattice, $m = 0.05, g = 1.0 \to m_B = 0.33(1), m_F = 0.35(2)$
- MLP with 2 inner layers

Larger networks give better vector fields



- 6×6 lattice
- $m = 0.05, g = 1.0, \mu = 0.5$

Future

- Scalable control variates for fermion sign problems
- Application of control variates to S2N problems
- Continue to check the applicability of contour deformation methods

Thank you!

Constraints on manifolds[7]

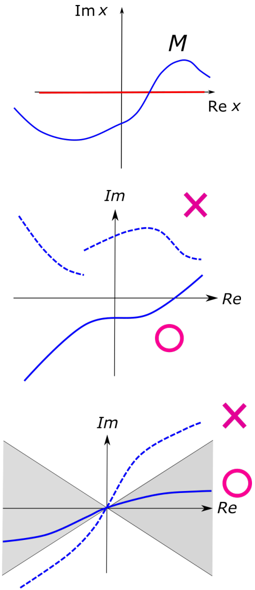
Manifolds give the correct $\langle\mathcal{O}\rangle$

$$\langle\mathcal{O}\rangle = \frac{\int_{\mathbb{R}} dy\ e^{-S(y)}\mathcal{O}(y)}{\int_{\mathbb{R}} dy\ e^{-S(y)}} = \frac{\int_{\mathcal{M}} dz\ e^{-S(z)}\mathcal{O}(z)}{\int_{\mathcal{M}} dz\ e^{-S(z)}}$$

when:

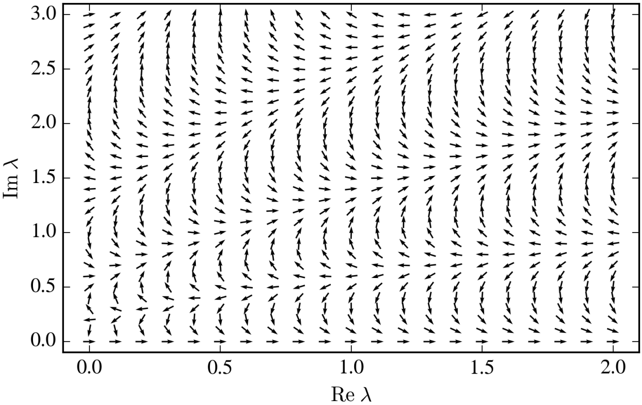
- The manifold (—) is a continuous manifold
- The manifold (—) is in "asymptotically safe" region
- Both e^{-S} and $e^{-S}\mathcal{O}$ are holomorphic functions in the region between (—) and (—)

→ **Cauchy's integral theorem!**



[7] A. Alexandru et al., Phys. Rev. D. 98, 034506(2018)

Zeros(?) of the partition function



- $m = 0.5$, 8×8 lattice
- 0 internal layer = linear transformation