Critical Temperature from (Un)supervised Deep Learning Autoencoders

`arxiv: 1903.03506`

Srijit Paul

Johannes Gutenberg University, Mainz

Machine Learning for High Energy Physics, on and off the lattice
ECT* Trento

Outline

Motivation

Physics goals

- Conventional MCMC algorithms $\rightarrow$ Critical slowing down.$\rightarrow$ Difficulty in pinpointing T_C.
- Observables with Finite Volume effects.

Algorithmic goals

- Understand domain of applicability of autoencoders.
- Limitations.

Motivation

Physics goals

- Conventional MCMC algorithms $\rightarrow$ Critical slowing down.$\rightarrow$ Difficulty in pinpointing T_C.
- Observables with Finite Volume effects.

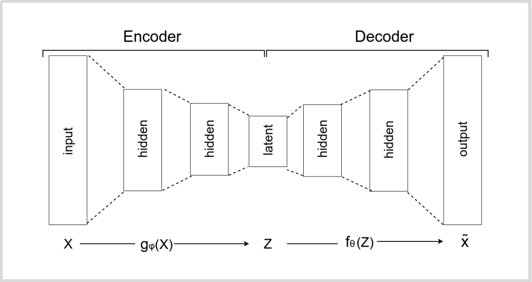
Algorithmic goals

- Understand domain of applicability of autoencoders.
- Limitations.

Deep Learning Autoencoders

Objective: Learning features in a given dataset hierarchically.

- Autoencoders (AE): Dimensionality reduction.



- Variational Autoencoders (VAE): Learn parameters of $X = P(\phi)$ distribution.

[S. Wetzel's talk]

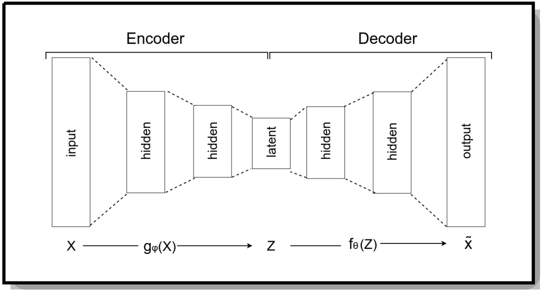
- VAE with convolutional layers.

[M. Cristoforetti's talk]

Deep Learning Autoencoders

Objective: Learning features in a given dataset hierarchically.

- Autoencoders (AE): Dimensionality reduction.



- Variational Autoencoders (VAE): Learn parameters of $X = P(\phi)$ distribution.

[S. Wetzel's talk]

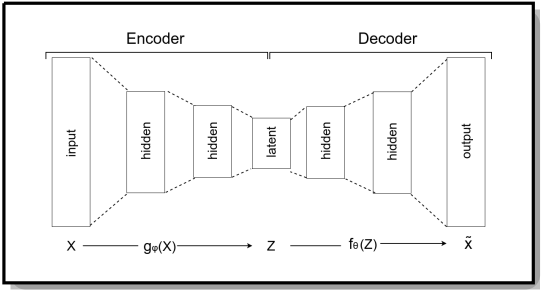
- VAE with convolutional layers.

[M. Cristoforetti's talk]

Deep Learning Autoencoders

Objective: Learning features in a given dataset hierarchically.

- Autoencoders (AE): Dimensionality reduction.



- Variational Autoencoders (VAE): Learn parameters of $X = P(\phi)$ distribution.

[S. Wetzel's talk]

- VAE with convolutional layers.

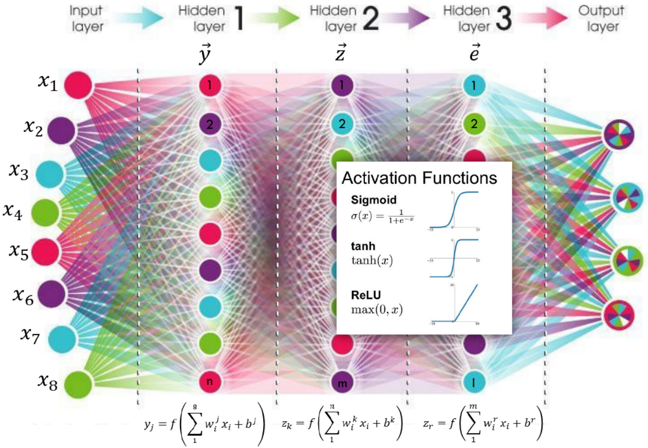
[M. Cristoforetti's talk]

Typical Neural Network

1. Input layer
2. Hidden layer
3. Hidden layer
4. Hidden layer
5. .
6. .
7. .
8. .
9. .

……..

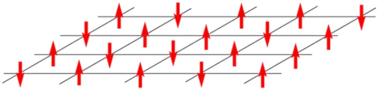
10. Output layer



Credits: neuralnetworksanddeeplearning.com 2016

Ising Model

- $1D$ Not so interesting: No phase transition (never magnetised)
- $2D$ more interesting: There is a phase transition
- Simplest Description of Ferromagnetism



- Hamiltonian:

$$H = -J \sum_{i,j=nn(i)}^{N} s_i s_j - \mu h \sum_{i=1}^{N} s_i$$

Nearest neighbors

Observables:

- Magnetization is the order parameter:

$$m = \frac{1}{N} \sum_{i=1}^{N} |s_i|$$

The 2D Ising model has a second order phase transition (magnetization is continuous)

- Magnetic susceptibility

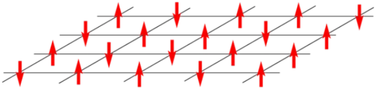
$$\chi = \frac{N}{T} \left(\langle m^2 \rangle - \langle m \rangle^2 \right)$$

- Heat Capacity

$$C = \frac{\partial \langle E \rangle}{\partial T}$$

Ising Model

- $1D$ Not so interesting: No phase transition (never magnetised)
- $2D$ more interesting: There is a phase transition
- Simplest Description of Ferromagnetism



- Hamiltonian:

$$H = -J \sum_{i,j=nn(i)}^{N} s_i s_j - \mu h \sum_{i=1}^{N} s_i$$

Nearest neighbors

Observables (near criticality $\sim T_c$):

- Magnetization is the order parameter:

$$m = \frac{1}{N} \sum_{i=1}^{N} |s_i| \qquad m(T) \sim |T - T_c|^b$$

The 2D Ising model has a second order phase transition (magnetization is continuous)

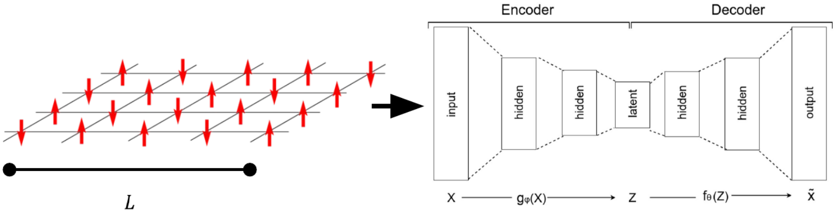
- Magnetic susceptibility

$$\chi = \frac{N}{T} (\langle m^2 \rangle - \langle m \rangle^2) \qquad \chi(T) \sim |T - T_c|^{-\gamma}$$

- Heat Capacity

$$C = \frac{\partial \langle E \rangle}{\partial T} \qquad \chi(T) \sim |T - T_c|^{-\alpha}$$

Ising with Autoencoder

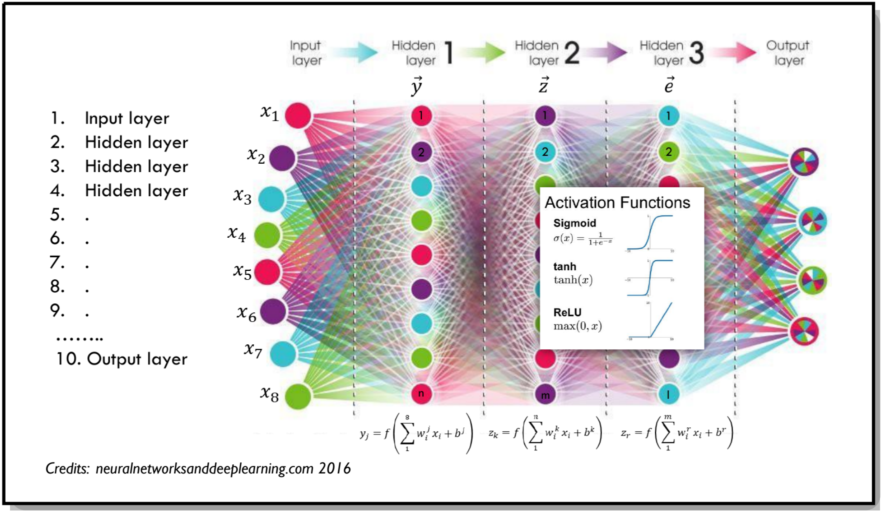


$$\mathrm{MSE}(\theta, \phi) = \frac{1}{n_{\text{data}}} \sum_{i=1} \left(X_i - f_\theta\left(g_\phi\left(X_i\right)\right)\right)^2$$

- $\tilde{X} = f_\theta\left(g_\phi\left(X\right)\right) \sim Id(X)$

Can we do away with layers/Activation functions?

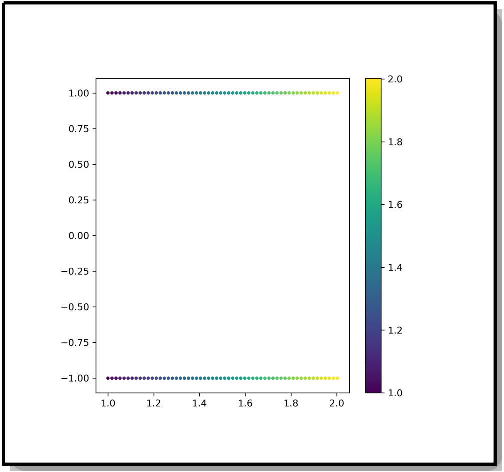
- Imagine 0 layers, 1 latent dimension. T = 1, 2.25, 4. Identity Activation function.



- Typical Latent dimension for T=1-2

Can we do away with layers/Activation functions?

- Imagine 0 layers, 1 latent dimension. T = 1, 2.25, 4. Identity Activation function.
- Typical Latent dimension for T=1-2.



- Same network can't be trained over a range of T

Can we do away with layers/Activation functions?

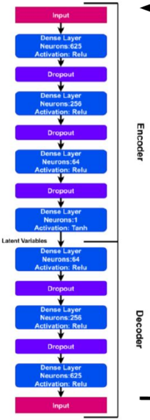
- Imagine 0 layers, 1 latent dimension. T = 1, 2.25, 4. Identity Activation function.
- Typical Latent dimension for T=1-2.
- Same network can't be trained over a range of T
- Need Activation to switch on and off a particular neuron for configurations of different temperatures.

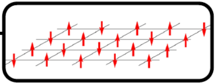
Can we do away with layers/Activation functions?

- Imagine 0 layers, 1 latent dimension. T = 1, 2.25, 4. Identity Activation function.
- Typical Latent dimension for T=1-2.
- Same network can't be trained over a range of T
- Need Activation to switch on and off a particular neuron for configurations of different temperatures.

Ising with Autoencoder

- Eight layers
- Fully connected (Dense)
- **Single** latent dimension
- Through experimentation



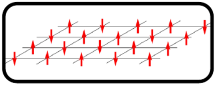


$$\text{relu} : y = max(0, x) = \begin{Bmatrix} x, & \text{if } x > 0 \\ 0 & \text{if } x \leq 0 \end{Bmatrix}$$

$$\tanh : y = \frac{1 - e^{-2x}}{1 + e^{-2x}}$$

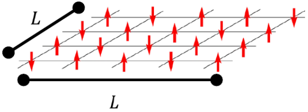
Dropout, reduces overfitting

G. E. Hinton et al, arXiv:1207.0580.



Ising with Autoencoder

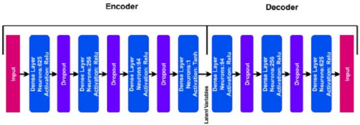
- Each configuration is re-expressed in the form of a vector:



L^2

(-1, 1, -1,1,1, -1,1,-1,1,-1,1,1,-1,1,-1,1,1,1,1,-1)

Input into the encoder



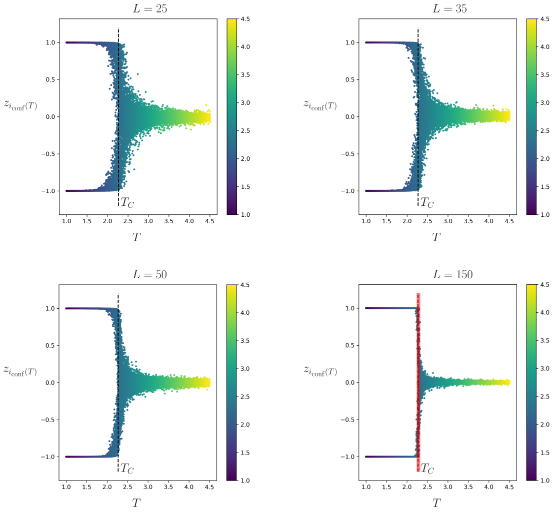
$z_{i_{\mathrm{conf}}}$

Latent Dimension

- In other words, each configuration is assigned a number, the latent dimension, which includes all the physically necessary information so that the decoder re-creates the actual configuration

Our setup

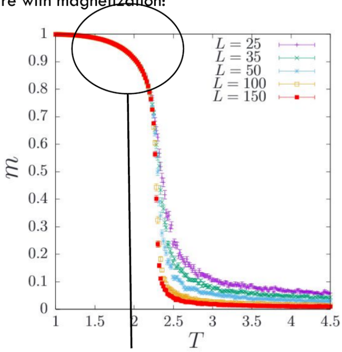
$40,000$ configs, $2/3$ training, $1/3$ validation.



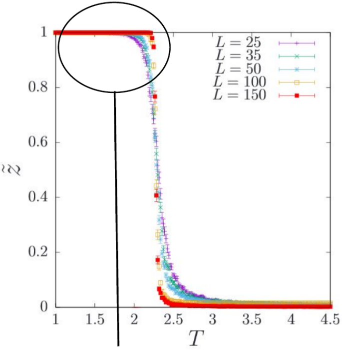
Order parameter & Pseudo-order parameter

$$m = \frac{1}{N_{\text{conf}}} \sum_{i=1}^{N_{\text{conf}}} |s_i| \qquad \tilde{z} = \frac{1}{N_{\text{conf}}} \sum_{i=1}^{N_{\text{conf}}} |z_{i_{\text{conf}}}|$$

Compare with magnetization:



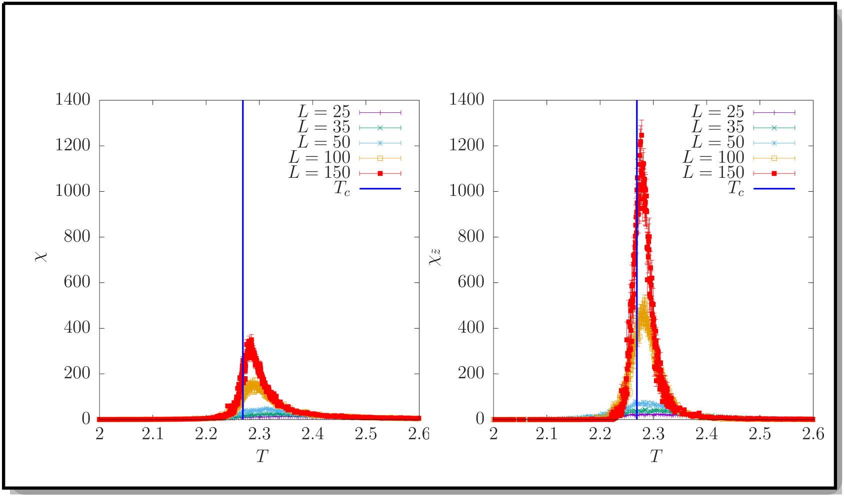
Second order



As if First order

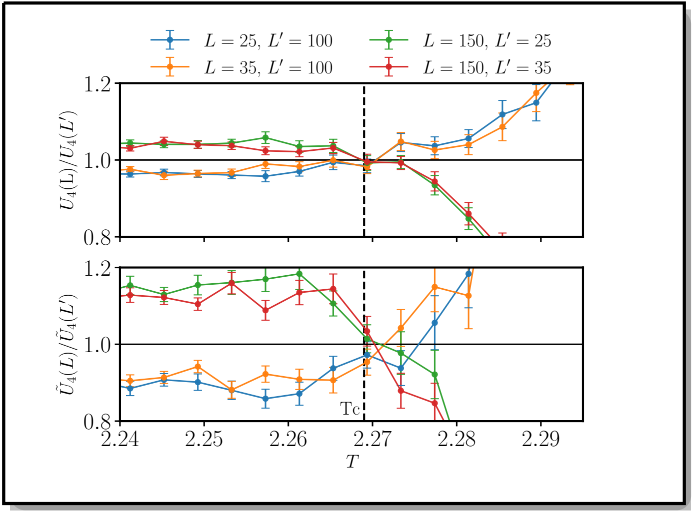
Susceptibility & Latent Susceptibility

$$\chi = \frac{L^2}{T}\left(\langle m^2\rangle - \langle m\rangle^2\right) \qquad \chi_{\tilde{z}} = \frac{L^2}{T}\left(\langle \tilde{z}^2\rangle - \langle \tilde{z}\rangle^2\right)$$



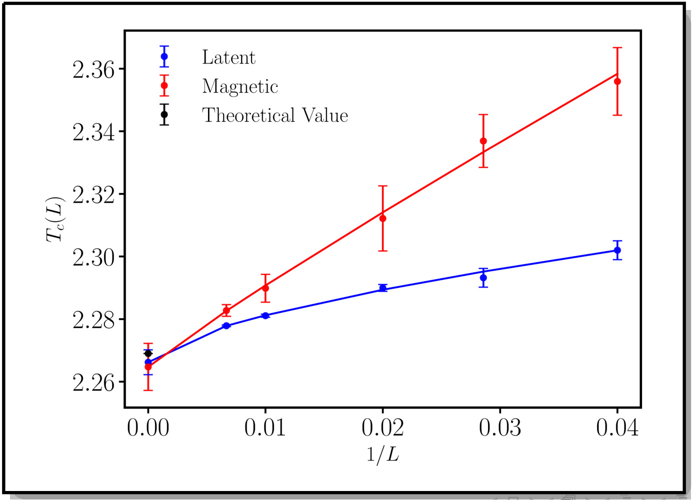
Extracting the T_C

$$U_4 = 1 - \frac{\langle m^4 \rangle}{3\langle m^2 \rangle^2} \qquad \tilde{U}_4 = 1 - \frac{\langle \tilde{z}^4 \rangle}{3\langle \tilde{z}^2 \rangle^2}$$



Extracting the T_C

- Noisy Binder Cumulant ratios, first indication that issues in Finite Size Scaling.
- Extracted T_C from $\chi_{\tilde{z}}$ peaks.



Takebacks

$$T_c(L) - T_c(L = \infty) \propto L^{-1/\nu}$$

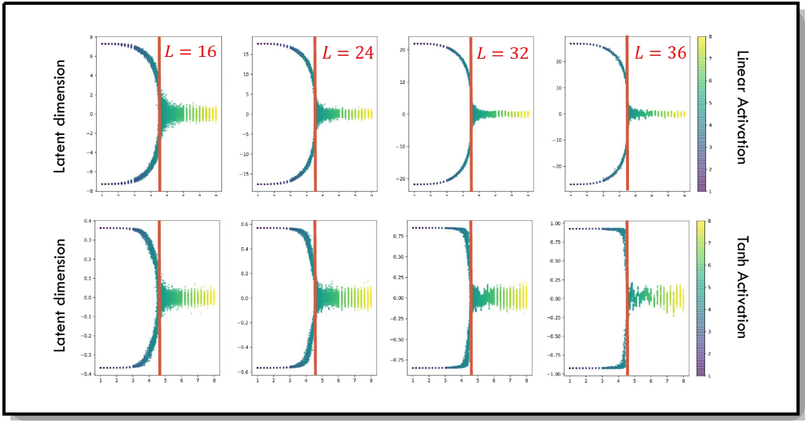
Susceptibility	$T_c(L = \infty)$	ν	$\chi^2/$ dof
Magnetic	$2.265(8)$	$1.08(20)$	0.15
Latent	$2.266(4)$	$1.60(14)$	0.41

- Critical temperature can be extracted to adequate accuracy.
- Observed $\mathcal{Z}_2$ symmetry broken.
- Configurations from latent dimension are from a different universaity class, but share the same $T_C(\infty)$.
- Latent dimension suffers from small finite volume effects, can help in constructing observables with small FV effects.

3D Ising Model

$T_C = 4.511$, Second order.

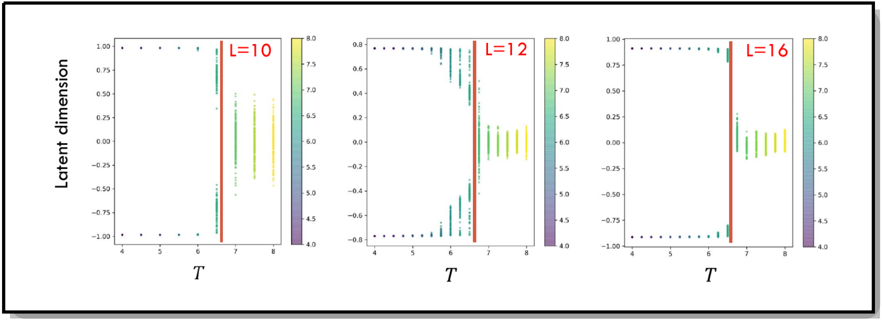
[*Talapov & Blöte 1996*]



4D Ising Model

$T_C = 6.65.$

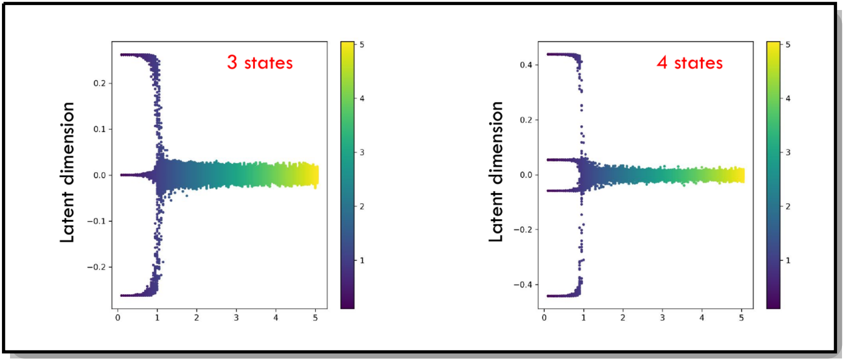
[*Lundow & Markström 2012*]



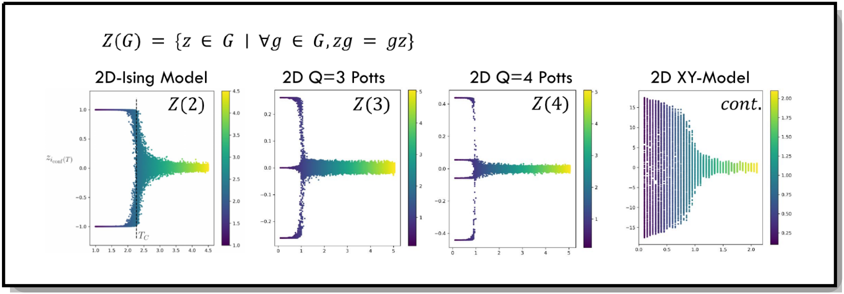
Potts Model

$T_C = 1.005$. $q \leq 4$ second order, $q > 4$ first order.

[*Wu 1982*]



Summary



- Autoencoders detect broken center symmetry of the underlying group.
- Significant effects of the choice of activation functions on the order of the phase transition.

Outlook

- Need to test on theories whose order parameters are not a moment of the field variable.
- Investigate energy dependent loss functions.
- Looking forward to gauge theories.

Thanks to all my collaborators: Andreas, Dina, Charis, A. Apseros, C. Havadjia, S. Shiakas and D. Vadacchino.