Feature extraction of machine learning and phase transition point of Ising model

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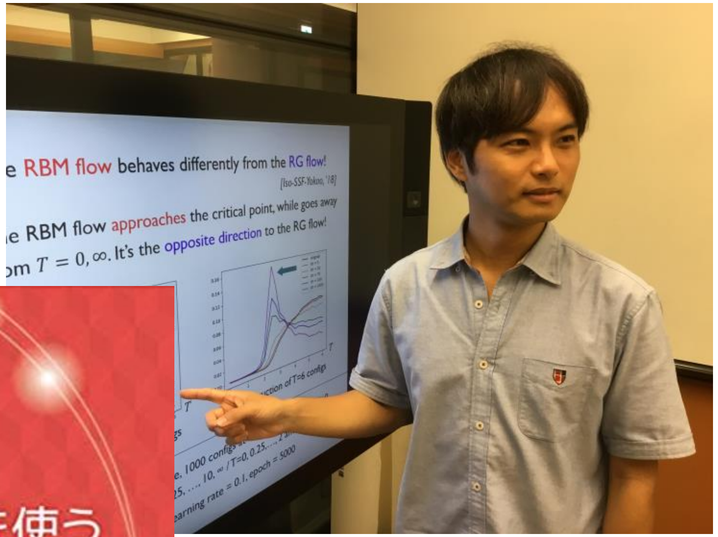
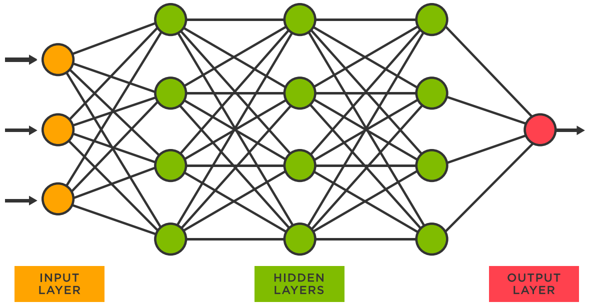
Shotaro Funai’s research theme:

What is the “feature” of data
which AI (machine learning) digitizes?
I want to understand it, hopefully using
some concepts of physics!

Edited by
Koji Hashimoto



Shotaro Funai



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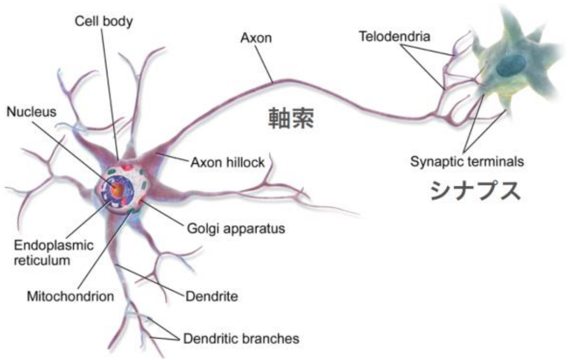
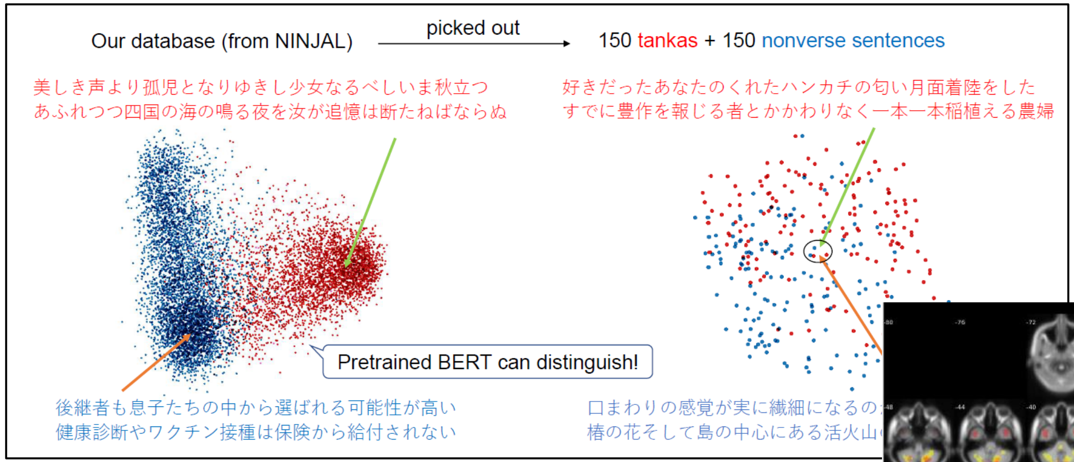


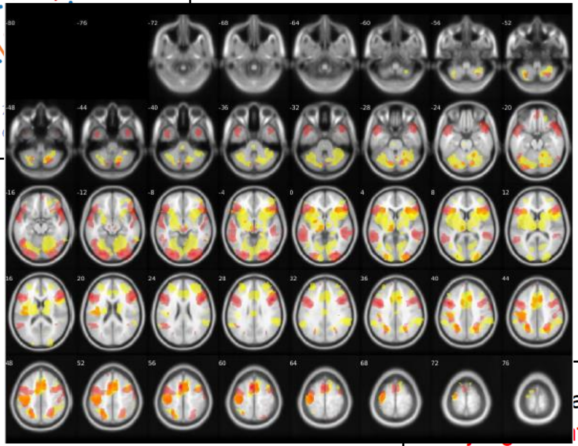
If we can regard AI as a toy model of brain or consciousness,
we might create “physics of consciousness”…?

Research 1: Can AI appreciate Japanese tankas (very short poems)?

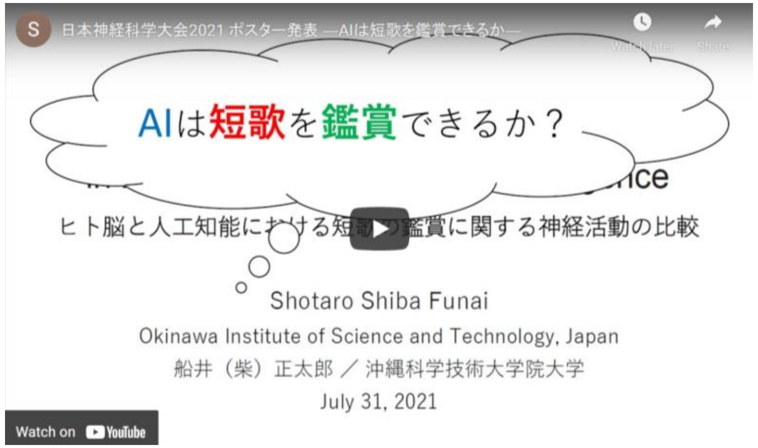
(at I-URIC, Inter-University Research Institute Corporation)



We analyze the BERT vectors (“features”) of tankas.



We measure human brain activities when they read tankas, and compare them with the BERT vectors.



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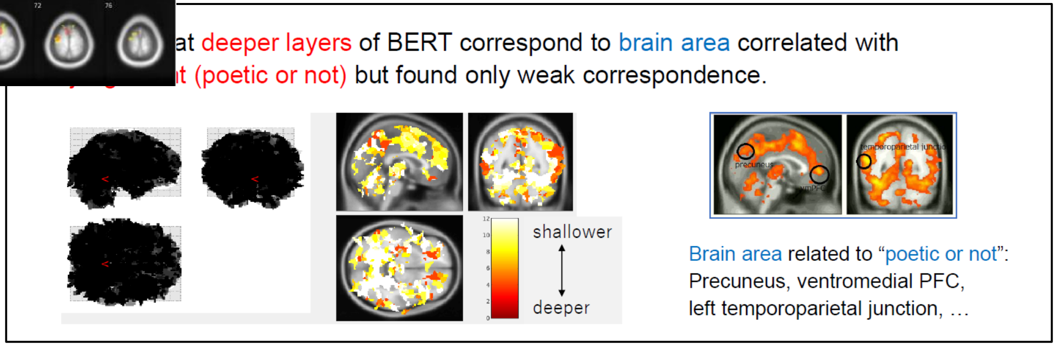
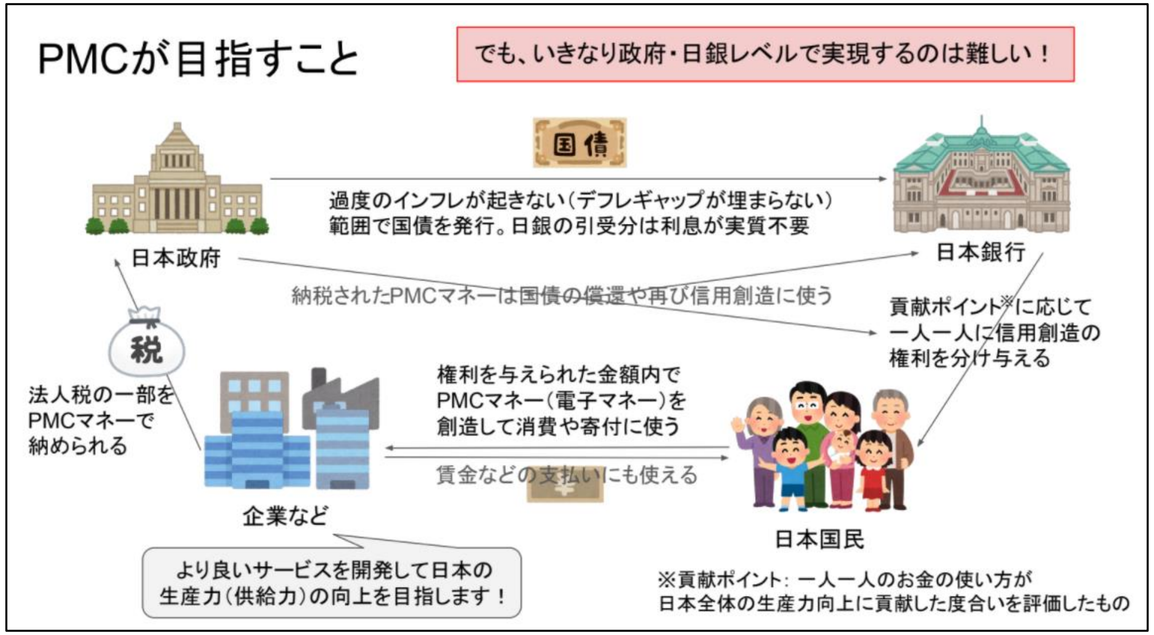


Research 2: New mechanism of money with AI

(at Keio University, SFC research institute)

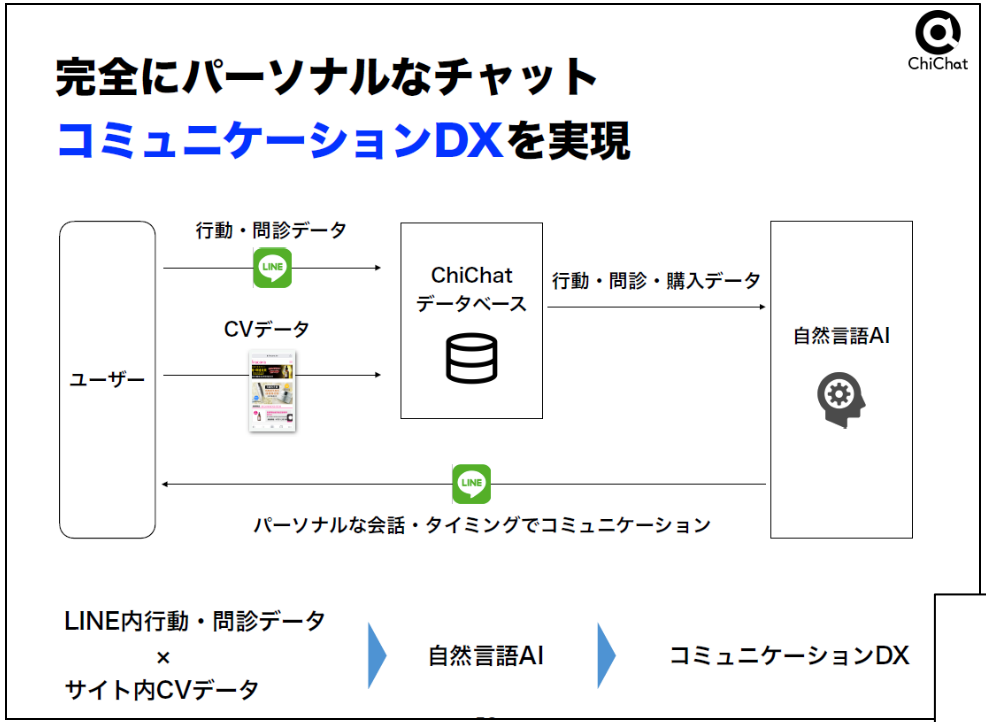


Japan has suffered from deflation for over 20 years!
Inflation targeting or helicopter money can solve it...?
With a new mechanism of money (PMC, personal money creation), let us make a wealthier society.

松田政策研究所での対談・鼎談

作家さとうみつろうさんとの対談

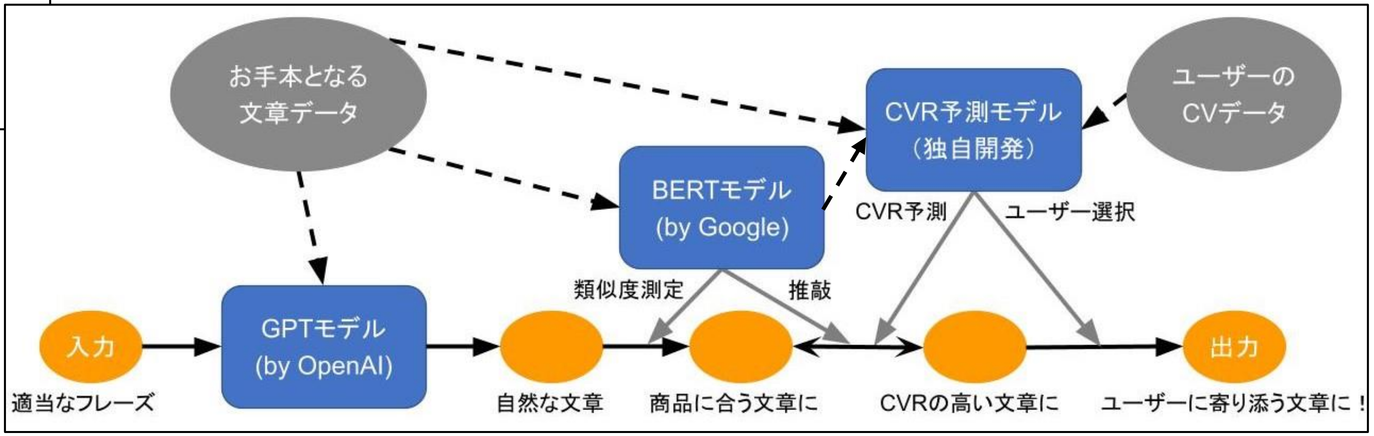
Research 3: Text generation for e-commerce (at Hitobito Inc.)



Goal for CEO (Ishikawa-san) is…

We want to develop an AI system which gets close to each user and generates messages so that the users can buy goods pleasantly.

We develop such a system using BERT and GPT, and their vectors ("features"). [Patent Pending]



Then, what is the “feature”…?

Research 4: Feature extraction of Ising model configurations

This talk

- We can discuss the “feature” using concepts of physics! (especially, renormalization)
- Ising model Hamilitonian:
  (in 1d or 2d square lattice)

$$\mathcal{H} = -J \sum_{\langle ij \rangle} s_i s_j - H \sum_i s_i$$

- Spin configurations at various temperatures (with $J = 1, H = 0$; white: $s_i = 1$, black: $s_i = -1$)

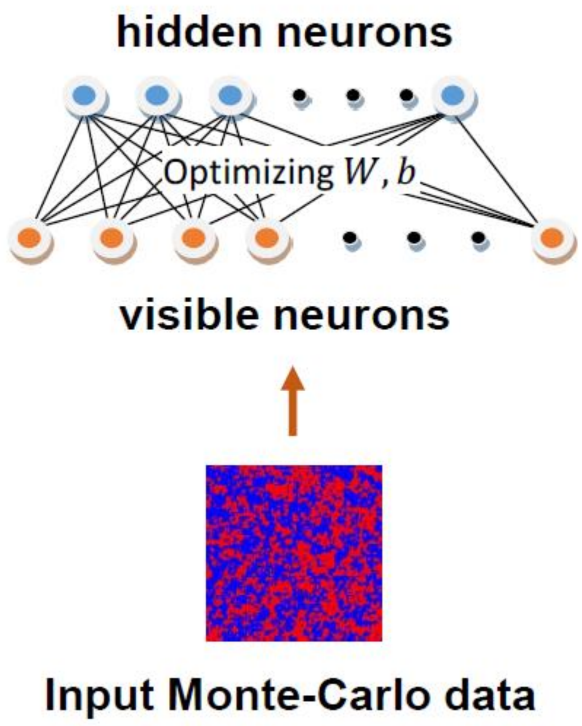
T=0.0 2.0 4.0 6.0 8.0 ...

phase transition at $T = T_c = 2.27$

[Iso-SSF-Yokoo, '18] [SSF-Giataganas, '18]

➢ Input data (which may be peculiar…)

- Spin configurations generated with Metropolis Monte Carlo simulation.
- Data includes the same number of configs at various temperatures (or external fields H) with constant interval, for example, $T = 0, 0.1, 0.2, \ldots, 9.9$ (100 temps).
- This choice may be *unnatural* in physical systems, but we chose them so that input data include various image patterns.
- Then, anyway, we can define and calculate probability distribution of configs (as images) in input data.



➢ We use the Restricted Boltzmann Machine (RBM)

- This type of a neural network is trained so that it outputs the configs with the *same probability distribution* as input data.
- In the training process, the RBM extracts "features" of input data.

- The probability of output configs is defined, using the “energy” function

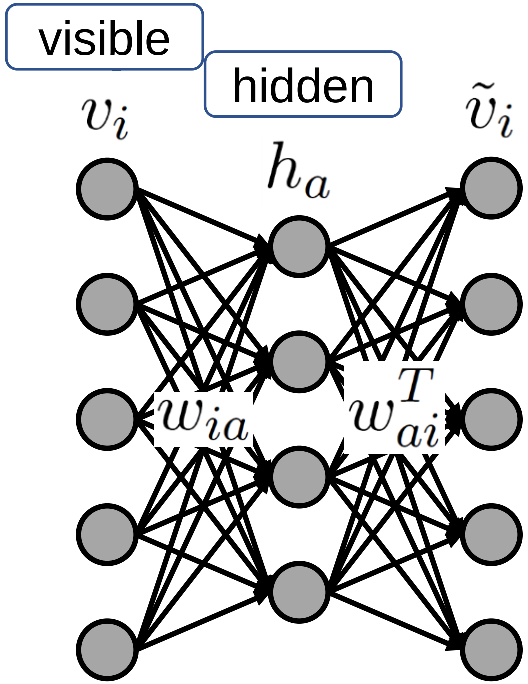
$$E(\{v_i\},\{h_a\}) = \sum_{i,a} v_i w_{ia} h_a + \sum_a b_a h_a + \sum_i c_i v_i$$

weights w_{ia}, bias b_a, c_i

by Boltzmann distribution

$$p(\{h_a\}) = \sum_{\{v_i\}} \frac{e^{-E(\{v_i\},\{h_a\})}}{\mathcal{Z}}$$

$$\tilde{p}(\{\tilde{v}_i\}) = \sum_{\{h_a\}} \frac{e^{-E(\{\tilde{v}_i\},\{h_a\})}}{\mathcal{Z}}$$



- We train the RBM (= optimize weights and bias) so that the KL divergence approaches a local minimum.

Loss function: $$\sum_{\{v_i\}} q(\{v_i\}) \log \frac{q(\{v_i\})}{\tilde{p}(\{v_i\})}$$

- KL divergence is a “distance” between two probability distributions:

$$\sum_{\{v_i\}} q(\{v_i\}) \log \frac{q(\{v_i\})}{\tilde{p}(\{v_i\})}$$

prob of an input image = v_i / prob of an output image = v_i

- In our experiment, the inputs are the spin configs $v_i = \pm 1$.
  The values of the hidden neurons are also binary: $h_a = \pm 1$.

- Then the expectation values of neurons are, using Boltzmann distribution,

$$\langle h_a \rangle = \tanh\left(\sum_i v_i w_{ia} + b_a\right)$$

$$\langle \tilde{v}_i \rangle = \tanh\left(\sum_a h_a w_{ai}^T + c_i\right)$$

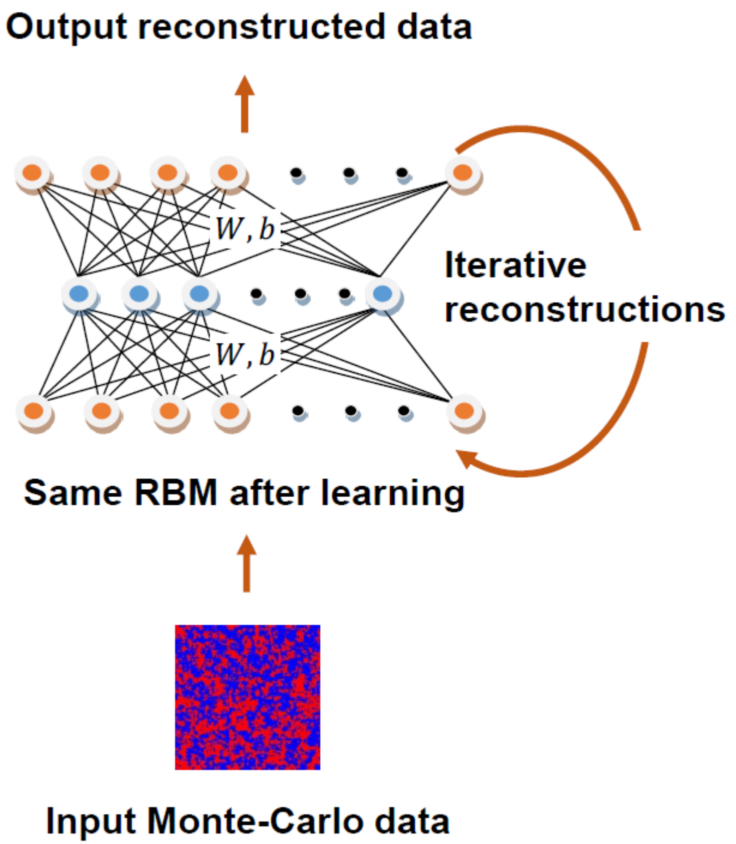
- The output (reconstructed) configs $\tilde{v}_i = \pm 1$ are obtained
  by replacing an expectation value $\langle \tilde{v}_i \rangle$ with a probability $(1 \pm \langle \tilde{v}_i \rangle)/2$.

To keep the same EV

- After the training finished, the probability distribution of input configs $q(\{v_i\})$ and that of output configs $\tilde{p}(\{v_i\})$ are similar but slightly different (since the KL divergence is *practically* not zero).

- If we input again the output configs, we obtain another probability distribution $\tilde{\tilde{p}}(\{v_i\})$ of reconstructed configs.

- Doing this iteratively, we get the flow of prob distribution of spin configs: $q(\{v_i\}) \to \tilde{p}(\{v_i\}) \to \tilde{\tilde{p}}(\{v_i\}) \to \ldots$



➢ Naïve questions:

1. Does this "RBM flow" correspond to the RG flow (renormalization group flow) of Ising model?

2. Does it have the fixed points describing the features? (The features should be *emphasized* along the RBM flow.)

Overview of our results

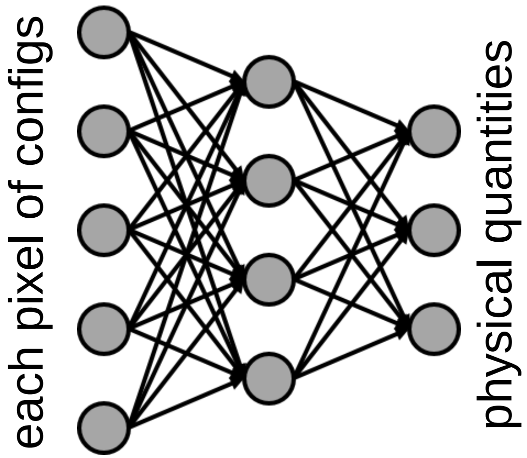
[Iso-SSF-Yokoo, '18]
[SSF-Giataganas, '18]

➢ The RBM flow *has* its fixed points in the (T, H) space.

- No fixed points of spin configurations exist;
  it is useful to generate *new* configs at the specific (T, H).
- To estimate (T, H) of the output configs, we use the following two ways:

1. We train *another* neural network to output correct (T, H) of input configs. (supervised learning)

   parameters of MMC simulation



2. For only the $H = 0$ configs, we can estimate T by calculating their energy.
   (We obtained the consistent results with method 1.)

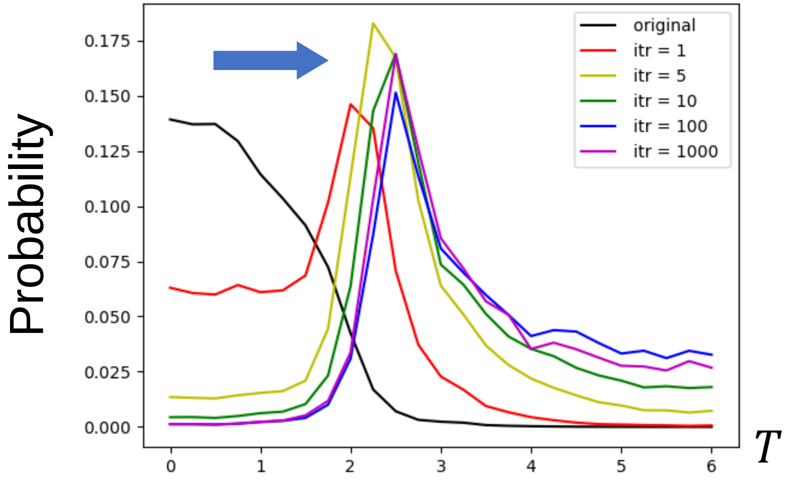
➢ The RBM flow behaves differently from the RG flow!

[Iso-SSF-Yokoo, '18]

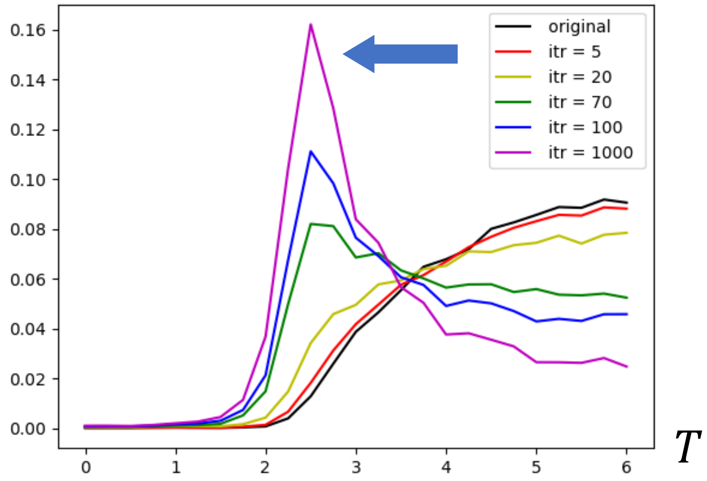
- The RBM flow *approaches* the phase transition point $T = T_c \sim 2.27$, while goes away from $T = 0, \infty$. It's the opposite direction to the RG flow!

2d, H=0

$n_h = 81$



Reconstruction of T=0 configs



Reconstruction of T=6 configs

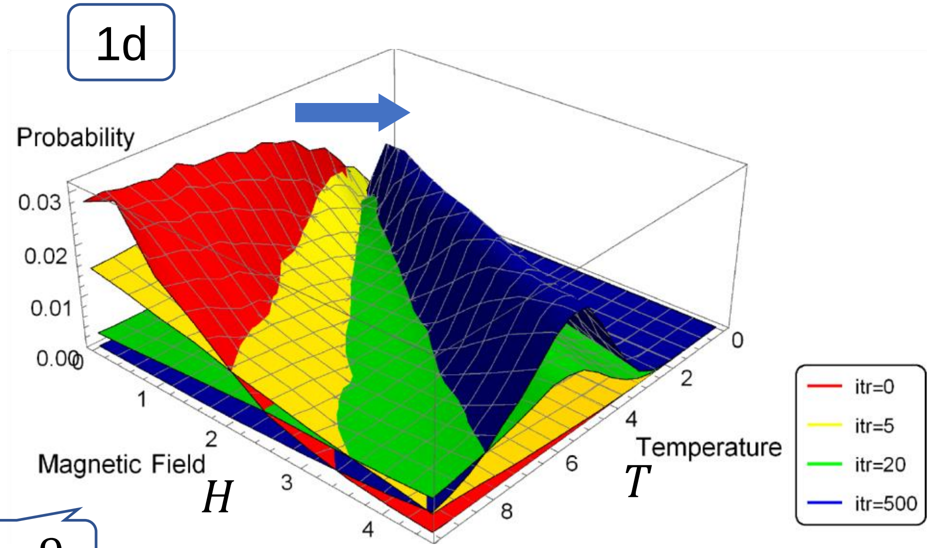
- Data: configs in 10x10 lattice, 1000 configs at each T=0, 0.25, …, 6, H=0.
  (Same results when T=0, 0.25, …, 10 / T=0, 0.25,…, 2 and 4, 4.25,…, 6.)

- RBM hyperparameters: $n_v = 100, n_h \leq n_v$, learning rate = 0.1, epoch = 5000

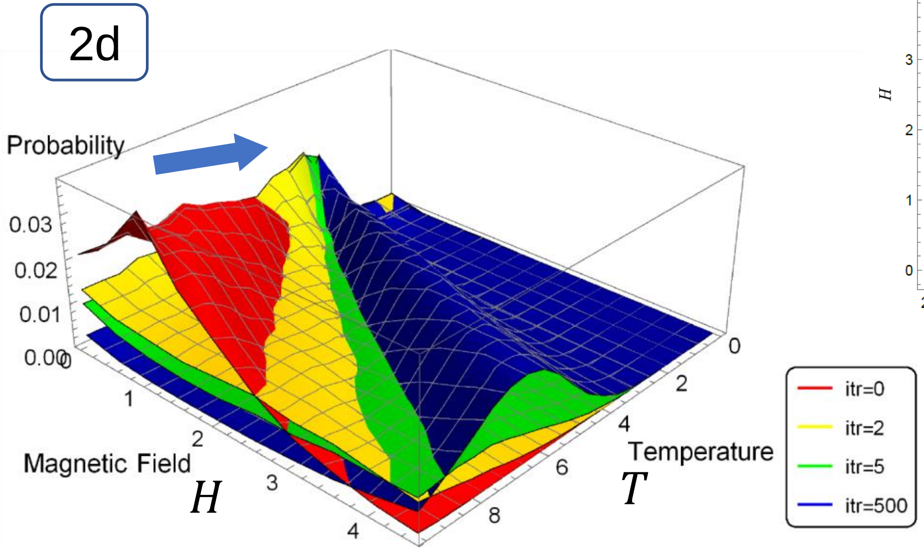
➢ For 1d and 2d Ising configs including $H \neq 0$ region:

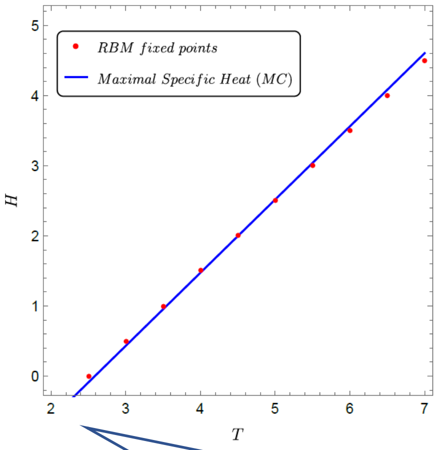
[SSF-Giataganas, '18]

- The RBM flow approaches the points with maximal heat capacity in (T, H) space.
  But the flow (and its fixed points) is different from the RG flow.



$n_h = 9$





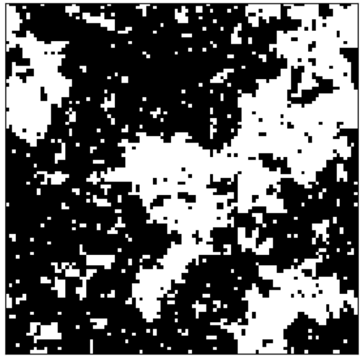
Includes
$T = T_c, H = 0$

- Data: configs in 100 (1d) or 10x10 (2d) lattice, 1000 configs at each (T,H), where T=0, 0.5, …, 9.5 and H=0, 0.5, …, 4.5.
- RBM hyperparameters: $n_v = 100, n_h \leq 16,$ learning rate = 0.001, epoch = 10000

This seems an interesting result, but…

- The reason is not clear: is it related to the scale invariance?
- The condition is also not clear: we need to study the parameter dependence.

Why and when is the RBM fixed point at $T = T_c$ (if $H = 0$) ?



Why? : Evidence for scale invariance

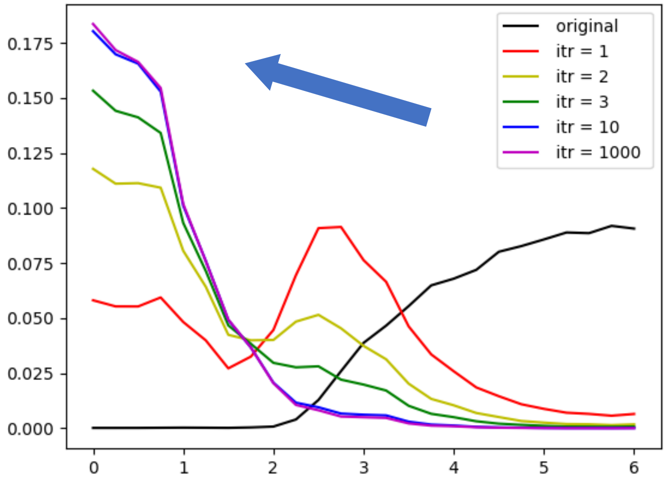
➢ Let us compare the two kinds of RBM by analyzing the RBM flows and their weights.

[Iso-SSF-Yokoo, ’18]

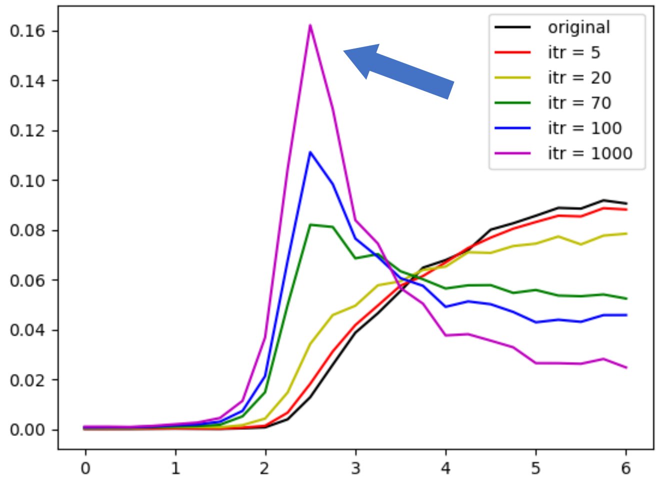
- One is the RBM trained by configs at only low temps.

With large scale

- The other is the RBM learning various temps $T = 0, 0.25, \ldots, 6$.



RBM learning only T=0



RBM learning T=0, …, 6

2d, H=0

low temp

high temp

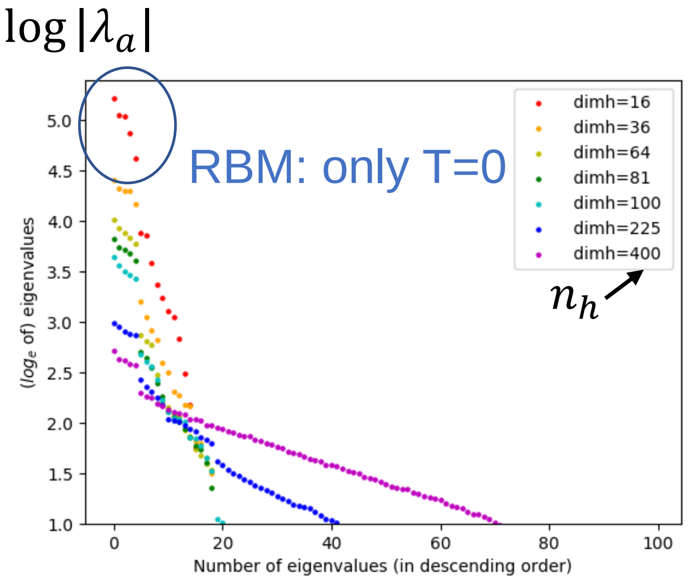
➢ Eigenvalues of weights $\sum_a w_{ia} w_{ja}$

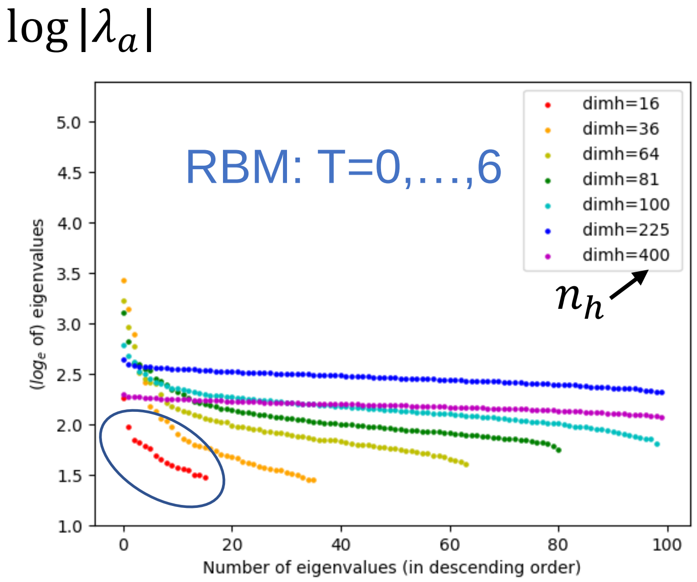
independent from basis of hidden neurons

$$ww^T u_a = \lambda_a u_a$$

- If the RBM learns configs at only low temps, only a few (~5) eigenvalues are especially large.
- If the RBM learns configs at $T = 0, 0.25, \ldots, 6$ (including high temp), all the eigenvalues have similar values.

  Many hidden neurons are needed to learn configs at various temps (=various scales).

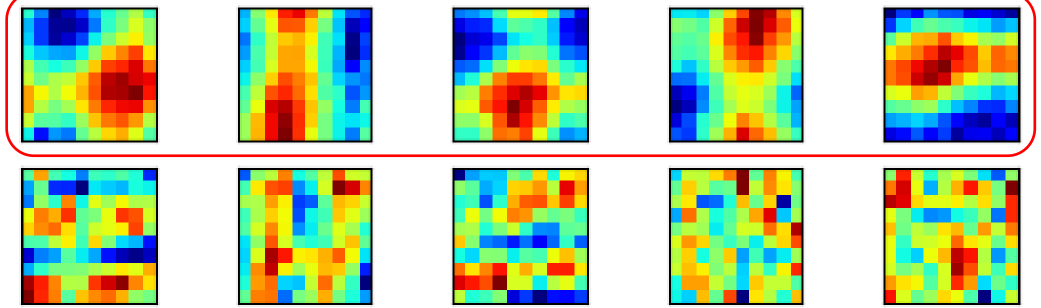




➢Eigenvectors of ww^T

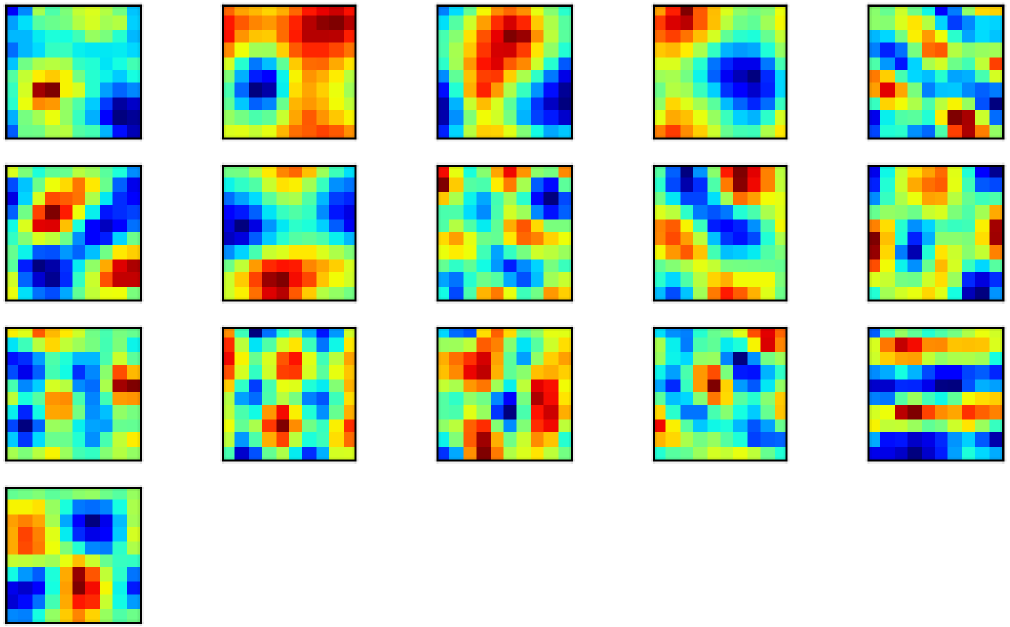
$$ww^T u_a = \lambda_a u_a$$

- RBM learning only low temps ($T = 0, \ldots, 2, n_h = 16$)



Configs with large scale have large eigenvalues.

- RBM learning various temps ($T = 0, \ldots, 6, n_h = 16$)



Configs with various scales have similar eigenvalues!

⬇

All of them appears in reconstructed images.

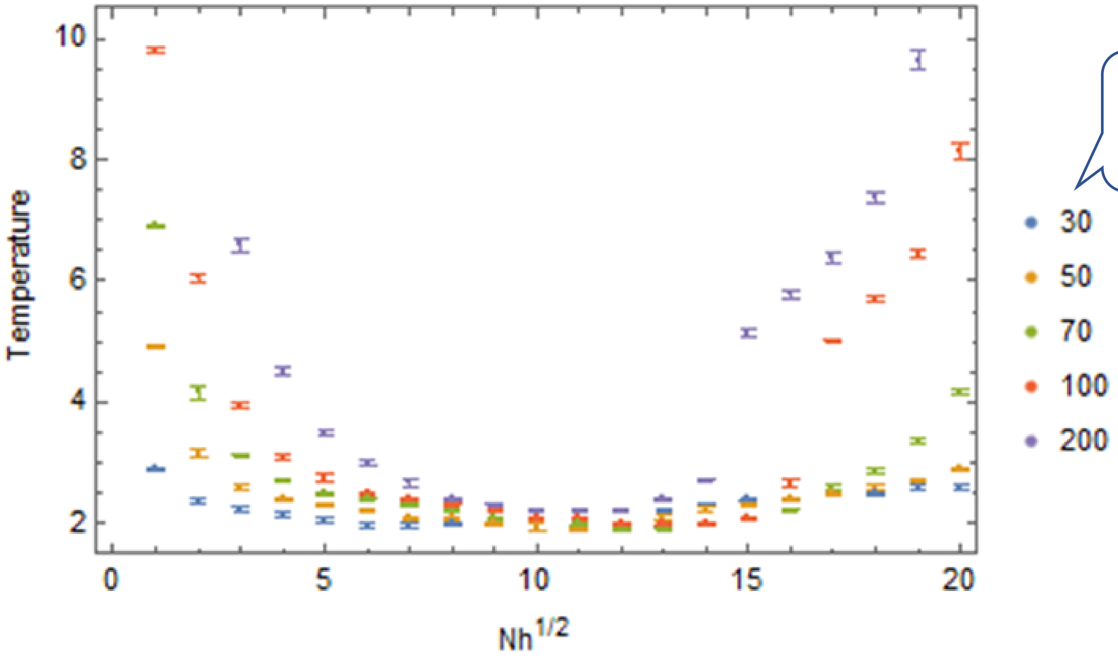
⬇

Scale invariance?

When? : The condition of parameters for $T \sim T_c$

[SSF, in progress]

Nv=20^2 (number of visible neurons, configs size)



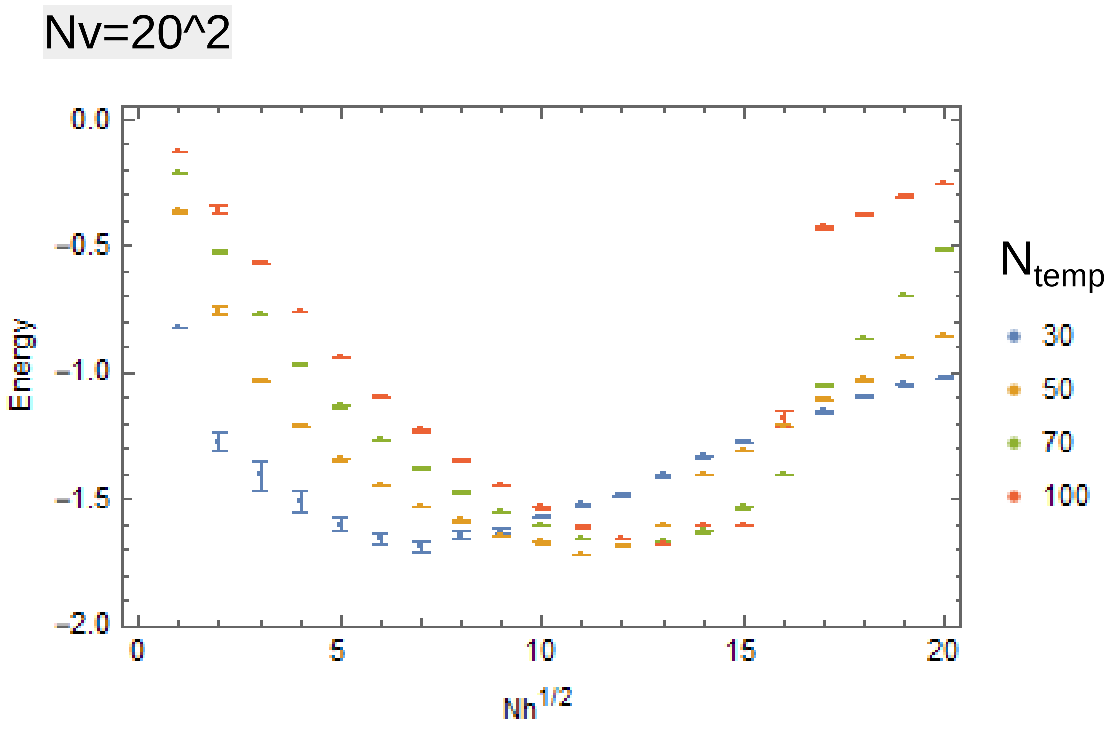
N_{temp}: input data include configs at $T = 0, 0.1, \dots, 0.1 \times (N_{temp} - 1)$

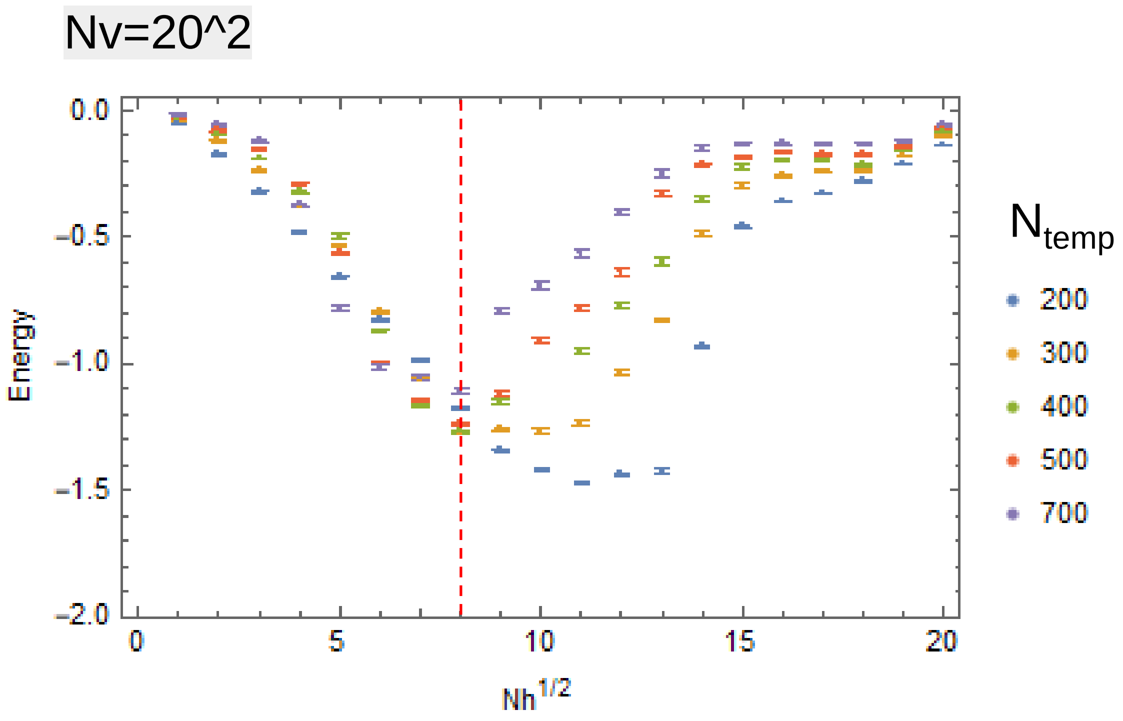
Around Nh/Nv = 1/4,
the RBM fixed point is
at the lowest temperature
and at $T \sim T_c$.

2d, H=0

Nh: number of hidden neurons

In terms of energy, instead of temperature, we find the result in more detail.





Nh with the minimum energy varies by N_{temp} (range of temps).

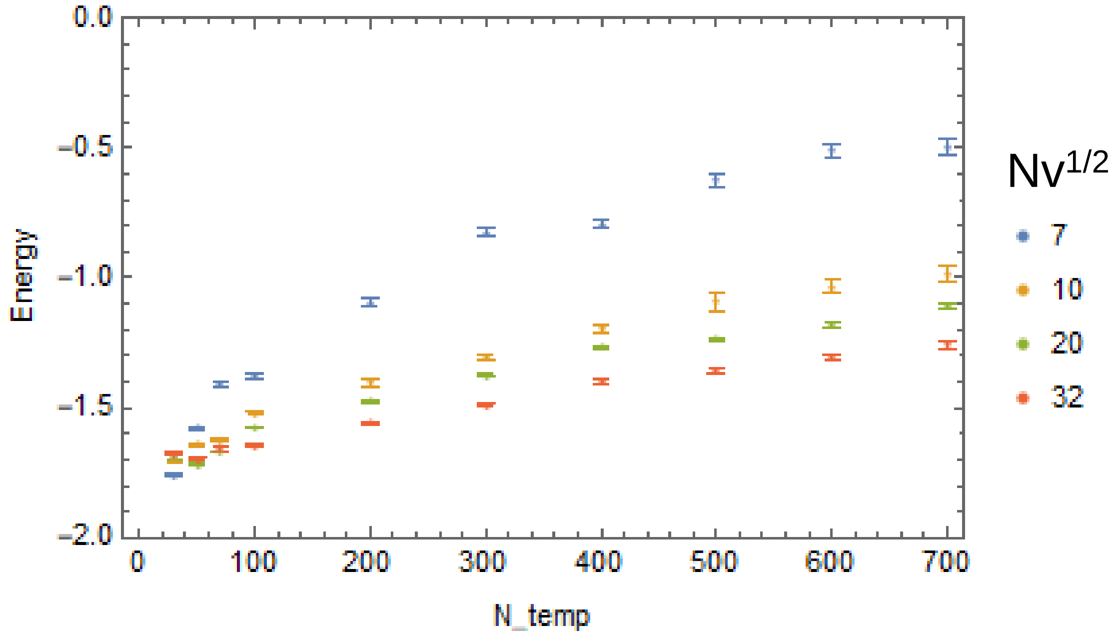
For large N_{temp}, Nh with the minimum energy seems to converge at Nh/Nv = 0.4^2.

Then, let us see the “minimum”, though we checked only Nh=$(\text{integer})^2$.

For larger size, the "minimum" energy of RBM fixed point goes up more slowly!

Nh fixed

"minimum" energy of RBM fixed point



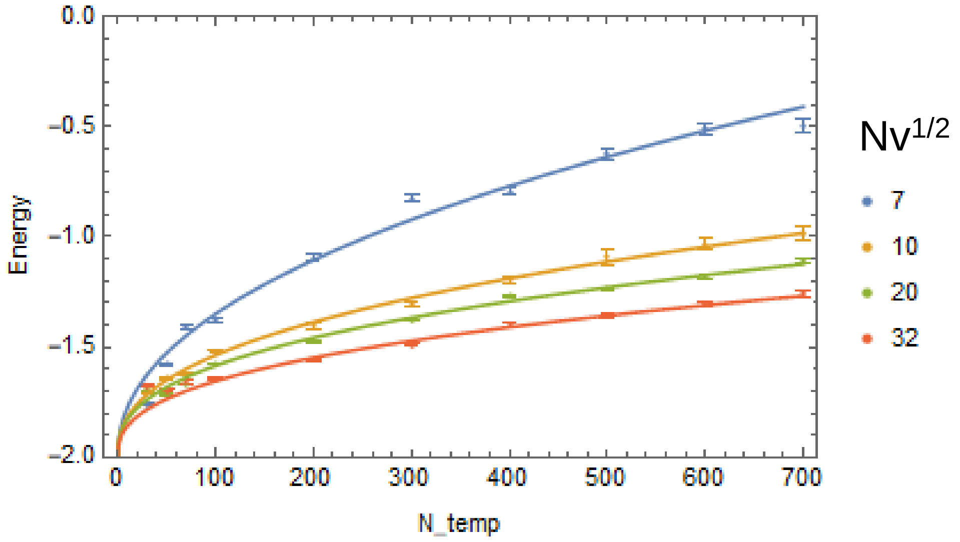
Nv: number of visible neurons, configs size
N_{temp}: input data include configs at
$T = 0, 0.1, \dots, 0.1 \times (N_{temp} - 1)$

From this plot, we can *presume* that

- For $N_{temp} \to \infty$ and Nv: fixed,
  the fixed point may be at $E \sim 0, T \to \infty$.
- For N_{temp}: fixed and Nv $\to \infty$,
  the fixed point may be at low energy.

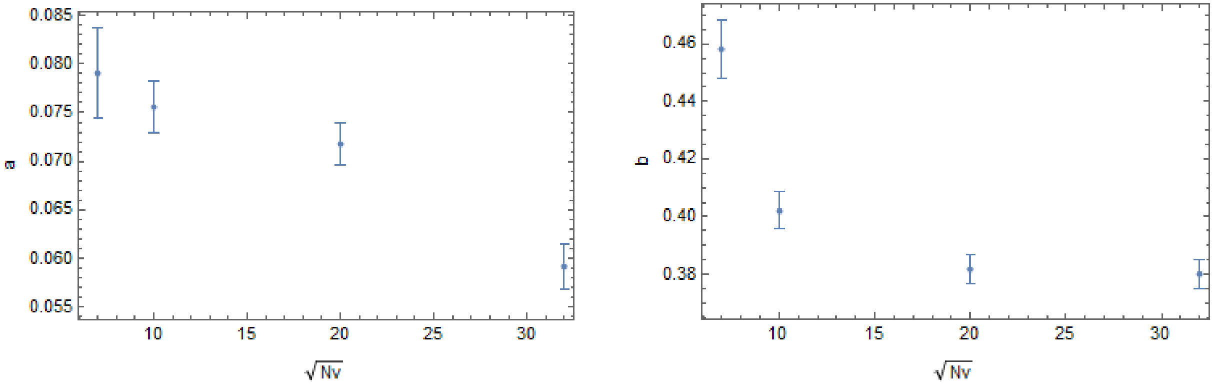
  Since at small N_{temp}
  the fixed point is at $E \sim -1.7, T \sim T_c$
  (as shown in the previous studies),
  the fixed point in this limit may be also
  at $T \sim T_c$.

If we try to fit these points to $\text{Energy} = -2 + a\, N_{temp}{}^{b}$, we obtain…



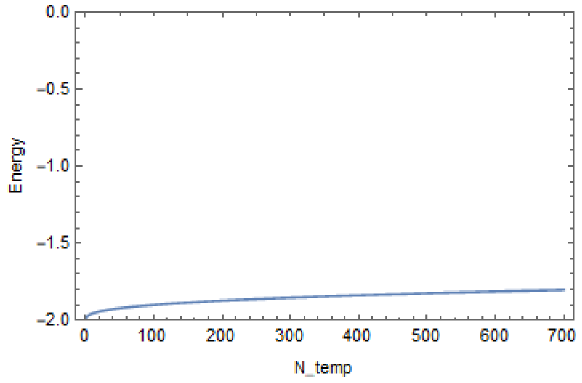
(Fitting for the points at $N_{temp} \geq 100$)

Plots of factors *a* and *b*



Both factors *a, b* decrease when Nv becomes larger.

It may suggest the plot of N_{temp} vs. Energy becomes more flat in Nv → ∞, like



Based on these observations, we can conjecture that the RBM fixed point is at $T \sim T_c$ when Nv is large enough (for fixed N_{temp}).

Finally, why is the RBM fixed point at smaller energy for larger Nv?

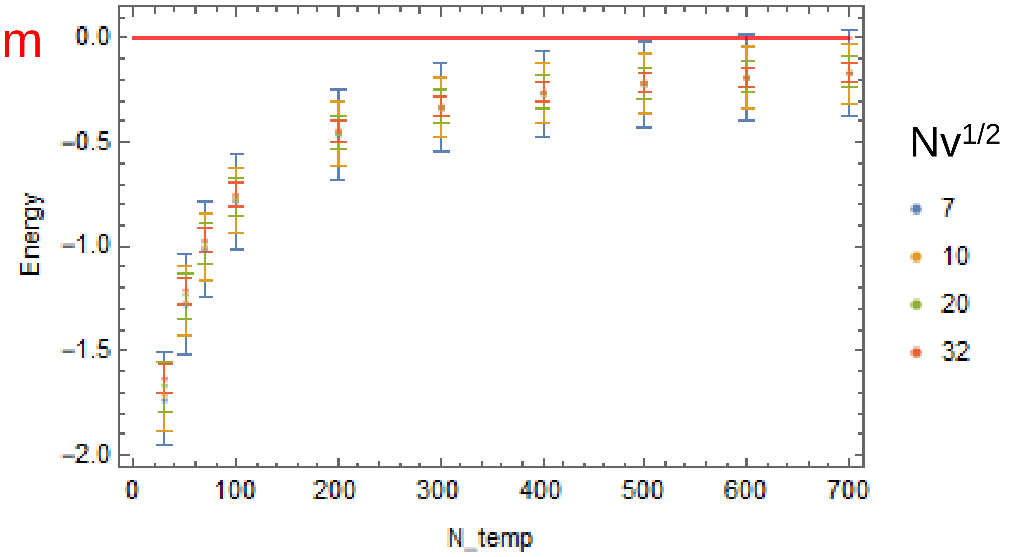
- It may be because the input data include the less random configurations.
- The less random configs we have, the more patterns RBM can learn!
- If only random configs are input, there is no way to reduce the loss of training RBM…

Averaged energy of input data (look at the error bars!):

It includes less random configs in larger Nv.

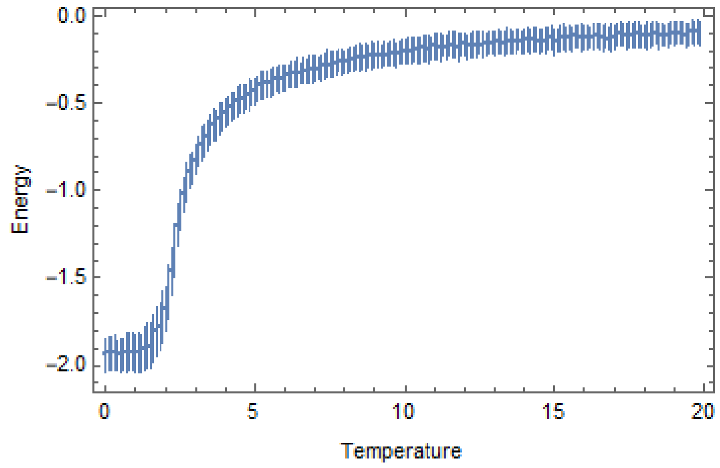
→ RBM can learn more patterns from non-random configs!

random



cf. energy of configs at fixed temp

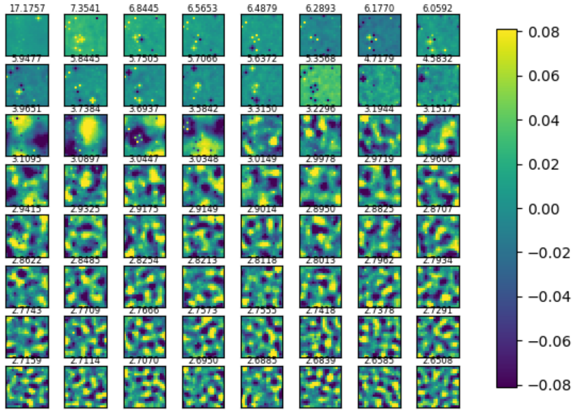
(Nv=20^2)



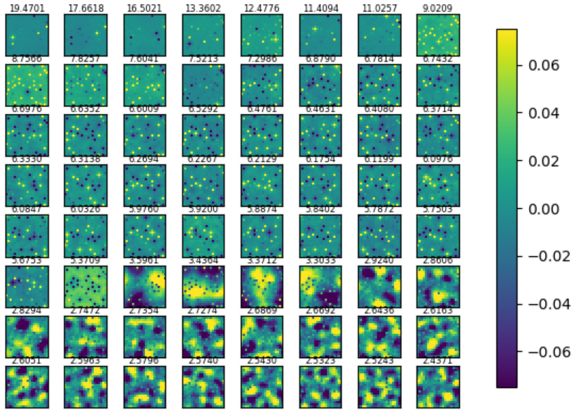
We can find the patterns that RBM learns in eigenvectors of weight matrix ww^T

(Nv=20^2 and Nh=8^2 are fixed below)

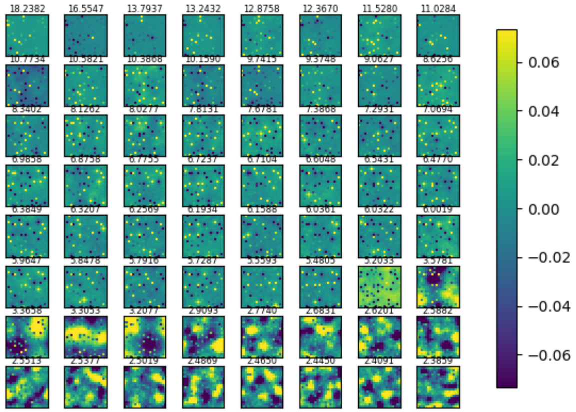
N_temp=200



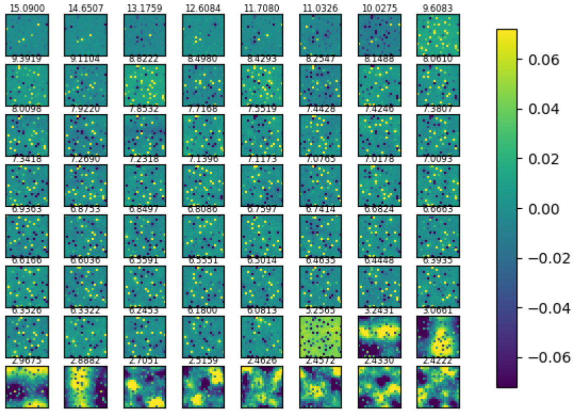
N_temp=300



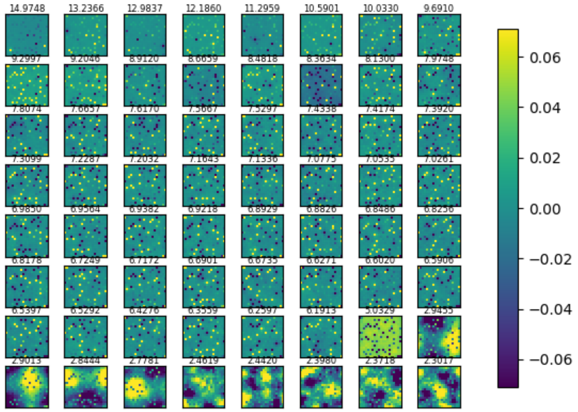
N_temp=400



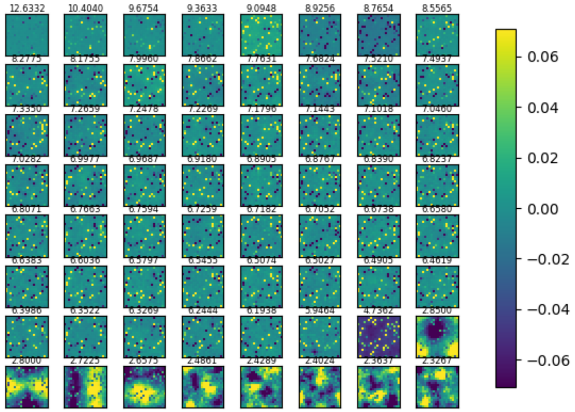
N_temp=500



N_temp=600



N_temp=700



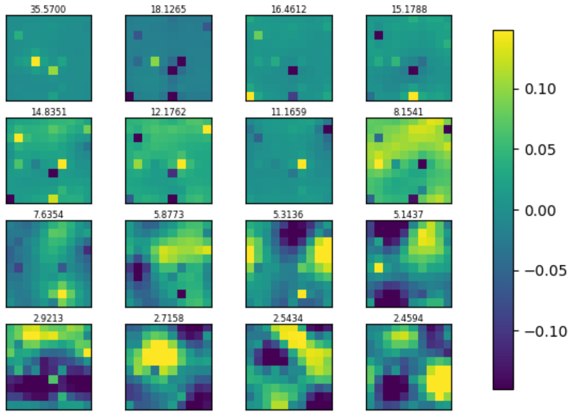
14%

9 of 8^2 eigenvectors show non-random patterns

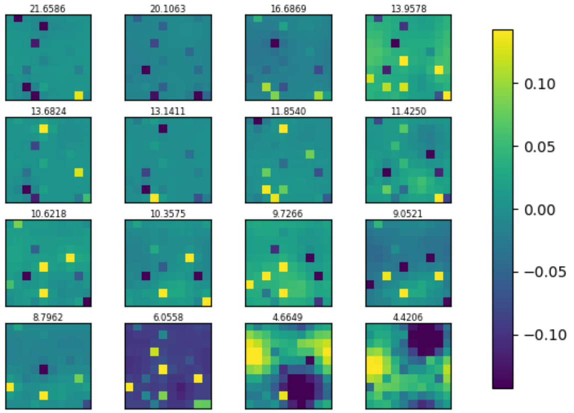
We can find the patterns that RBM learns in eigenvectors of weight matrix ww^T

(Nv=10^2 and Nh=4^2 are fixed below)

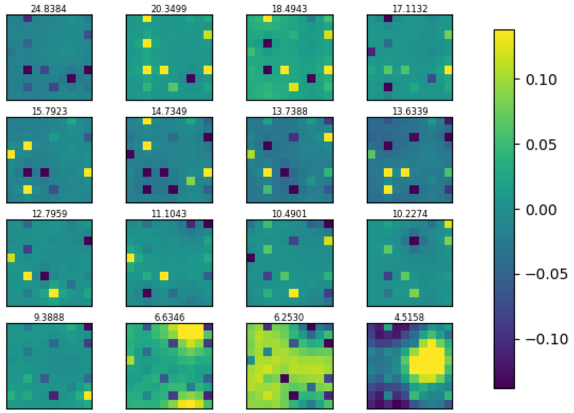
N_temp=200



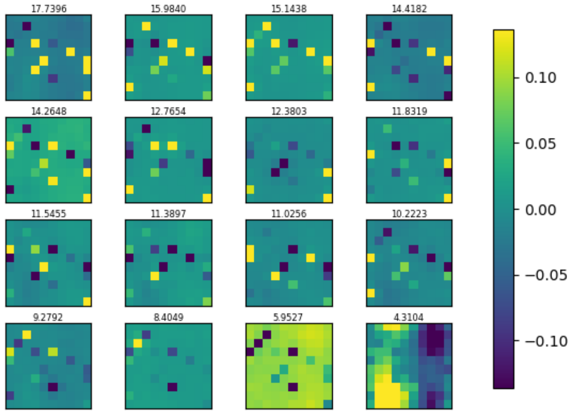
N_temp=300



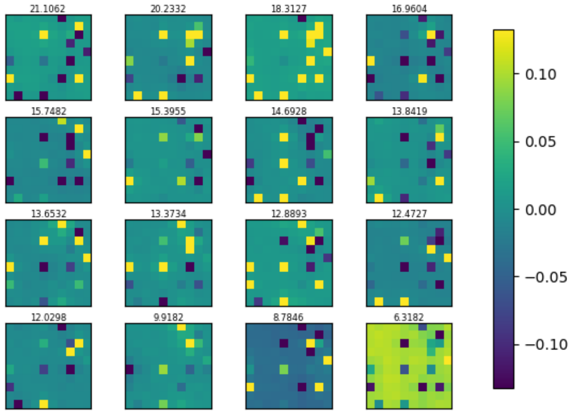
N_temp=400



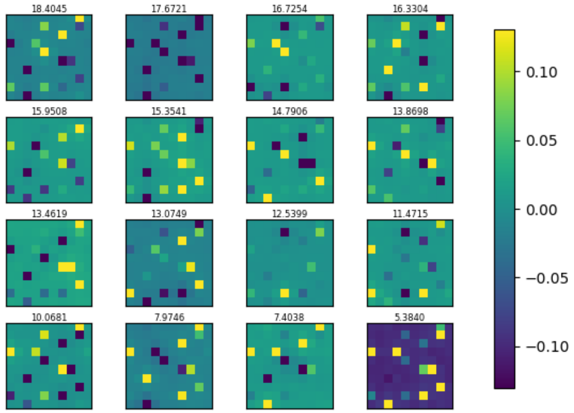
N_temp=500



N_temp=600



N_temp=700



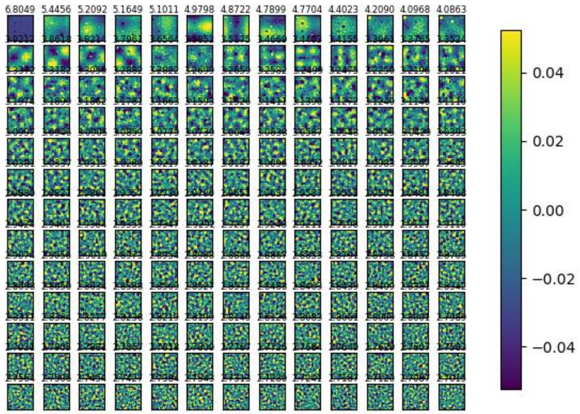
0%

no eigenvectors show non-random patterns

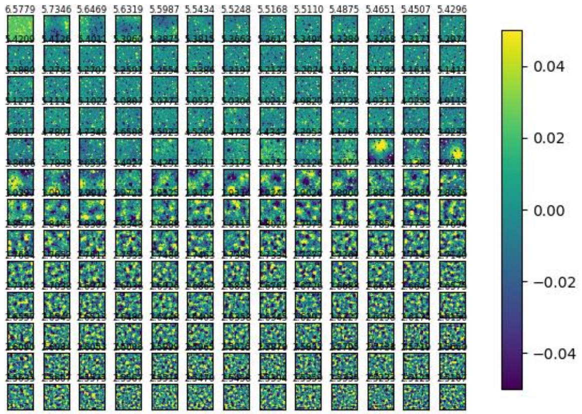
We can find the patterns that RBM learns in eigenvectors of weight matrix ww^T

(Nv=32^2 and Nh=13^2 are fixed below)

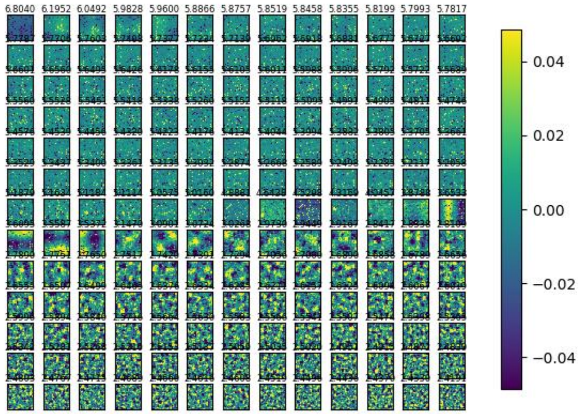
N_temp=200



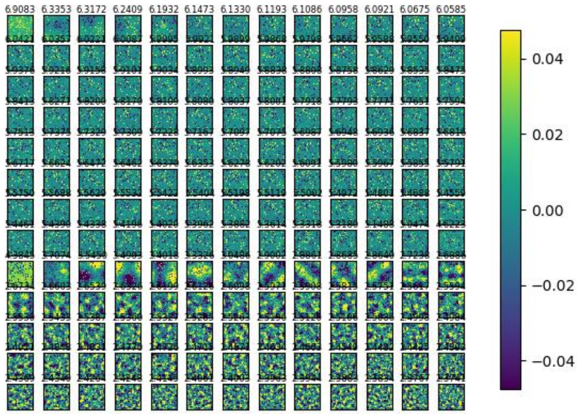
N_temp=300



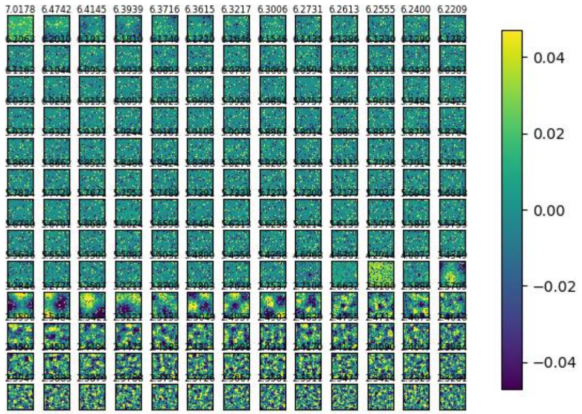
N_temp=400



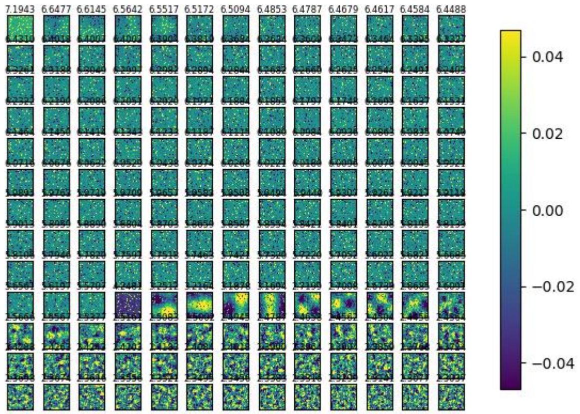
N_temp=500



N_temp=600



N_temp=700



28%

48 of 13^2 eigenvectors show non-random patterns

Conclusion

- We perform machine learning of RBM to extract features of spin configs in Ising model.
- We find that the RBM flow of reconstruction has the fixed point (= feature) just as the RG flow, but their behaviors are obviously different.
- We propose that the feature the RBM grasps may be the scale invariance (at phase transition point and maximal heat capacity).
- We also conjecture the condition of parameters (larger size, fixed N_{temp}) that the RBM fixed point is at phase transition point.