How phase transitions shape the learning of complex data in the Resctricted Boltzmann Machine



Bachtis et al NeurIPS '24 Rosset et al PRE '23

Aurélien Decelle – Universidad Complutense de Madrid





Madrid's group in Machine Learning



Giovanni Catania Beatriz Seoane AD

Lorenzo Rosset

Alfonso Navas Gomez

Paris-Saclay

PhD student Nicolas Béreux



<u>Paris-Saclay</u>

Cyril Furtlehner



ENS-Paris

Tony Bonnaire Giulio Biroli Dimitrios Bachtis







Machine Learning and generative model

Generative modelling is a quite common task when dealing with, for instance, Bayesian inference

$$p(\boldsymbol{\theta}|\mathcal{D}) = \frac{p(\mathcal{D}|\boldsymbol{\theta})p(\boldsymbol{\theta})}{Z(\mathcal{D})}$$

To infer/learn the parameters θ of some problem, we need to define the likelihood. \rightarrow the likelihood is a generative model

Machine Learning and generative model

Some approaches taken by modern Machine Learning is to

- \rightarrow use very « expressive » but not related to the data distribution (e.g. neural networks)
- \rightarrow bypass the need to compute the likelihood (e.g. Generative Adversarial Networks)

Others such as Diffusion Models (see Biroli's talk) are based upon a different setting.

Supervised vs Unsupervised

Machine Learning tasks are often categorized in three categories

- <u>Supervised Learning</u>
- Unsupervised Learning

A dataset of M elements in dimension N, with labels (a class or real value)

$$\{x_m\}_{m=1,\dots,M} \quad \{y_m\}_m$$
Example of classification $x = \overbrace{x_m} \\ y = \text{``cats''} \qquad \begin{array}{c} \text{Example} \\ \text{of} \\ y = \text{``cats''} \end{array} \quad \left(x,y\right) = \overbrace{y_m} \\ \text{egression} \\ \end{array}$

In both cases, we are looking to find the parameters of some function f that manage to predict the correct answer $f_{\theta^*}(x_m) = y_m$

Supervised vs Unsupervised

Machine Learning tasks are often categorized in three categories

- Supervised Learning
- <u>Unsupervised Learning</u>

A dataset of M elements in dimension N $\longrightarrow \{x_m\}_{m=1,...,M}$

Then, in most settings we want to **learn a probability distribution** matching the empirical one

Example of generative models

 $\hat{x} \sim p_{\theta^*}(x)$



Examples of clustering



Example of generative modelling

This models is part of what is usually called "Unsupervised learning" or Generative model. Its "purpose" is to learn a probability distribution based on a dataset. Examples:



automatic clustering

Define a <u>mixture model</u>: distribution \mathbf{P} \rightarrow learns its parameters



Non-exhaustive list of generative models



Diffusion models

Before...

Before I had to excuse myself for dealing with Boltzmann Machine when spealing about Machine Learning



Brief recall

<u>Hopfield model</u> : associative memory model \rightarrow it recalls « planted » patterns

- introduced by Hopfield in '82
- AGS '85 replica theory to recall when storing an extensive number of patterns
- Dreaming mechanism to increase the recall regime (Dotsenko Kanter, Sompolinski ~90', later Barra, Agliari et al. ~2019)
- More recently : Modern Hopfield model with exponential capacity

<u>The Restricted Boltzmann Machine</u> : generative model → it can generate new complex samples

- Smolensky '86, then popularized by Hinton with contrastive divergence ~2000
- It was use to extract features and train deep NN in ~2000 \rightarrow 2010
- Re-discovered by physicists ~2010 : Barra, Agliari, Monasson, ...
- Roots for energy-based models

The Restricted Boltzmann Machine from Hopfield to Hinton (and back?)

Recall on the Hopfield model (will be useful later) – we consider discrete spins $s_i = \pm 1$

$$\mathcal{H} = -\frac{1}{N} \sum_{i} J_{ij} s_i s_j = -\frac{1}{2N} \sum_{\mu} \left(\sum_{i} s_i \xi_i^{\mu} \right)^2$$
$$J_{ij} = \sum_{\mu} \xi_i^{\mu} \xi_j^{\mu}$$
$$\xi_i^{\mu} = \pm 1 \text{ with } p = 1/2 \text{ and } \mu = 1, \dots, P = \alpha N$$

The RBM : from Hopfield to Hinton (and back?)

<u>Order parameters</u>

 $\mathcal{H} = -\frac{1}{2N} \sum_{\mu} \left(\sum_{i} s_{i} \xi_{i}^{\mu} \right)^{2}$

$$m = \frac{1}{N} \sum_{i} \xi_{i}^{\mu} \langle s_{i} \rangle$$
$$q = \frac{1}{N} \sum_{i} \mathbb{E}_{\boldsymbol{\xi}} \left[\langle s_{i}^{a} \rangle \langle s_{i}^{b} \rangle \right]$$

Different phases

- P : Paramagnetic q,m=0
- R : Recall $q,m \neq 0$
- SG : Spin Glass $q \neq 0, m = 0$
- MR : Metastable Recall



From Hopfield to Bipartite architecture

$$p(\boldsymbol{s}) = \frac{1}{Z} \exp\left(-\beta \mathcal{H}[\boldsymbol{s}]\right)$$
$$= \frac{1}{Z} \int d\boldsymbol{\tau} \exp\left(-\boldsymbol{\tau}^2/2 + \sqrt{\frac{\beta}{N}} \sum_{i,\mu} s_i \xi_i^{\mu} \boldsymbol{\tau}_{\mu}\right) \longrightarrow \mathcal{H}_{\text{RBM}}[\boldsymbol{s}, \boldsymbol{\tau}] = -\sum_{i\mu} s_i w_{i\mu} \boldsymbol{\tau}_{\mu}$$
$$= \int d\boldsymbol{\tau} p_{\text{RBM}}[\boldsymbol{s}, \boldsymbol{\tau}]$$



Credit to Barra et al. 2018

From Hopfield to Bipartite architecture

 $\mathcal{H}_{\mathrm{RBM}}[oldsymbol{s},oldsymbol{ au}] = -\sum_{i\mu} s_i w_{i\mu} au_{\mu}$



linear response from the hidden layer Credit to Barra et al. 2018

From Hopfield to Bipartite architecture

 $\mathcal{H}_{ ext{RBM}}[oldsymbol{s},oldsymbol{ au}] = -\sum_{i\mu} s_i w_{i\mu} au_{\mu}$

What if we change the nature of the hidden nodes ? $\tau_a = \pm 1$

$$p(s_i | \boldsymbol{\tau}) = \tanh\left(\sum_{\mu} \xi_i^{\mu} \tau_{\mu}\right) \qquad \qquad \underline{\text{Distribution on the spins :}}$$
$$p(\tau_{\mu} | \boldsymbol{s}) = \tanh\left(\sum_{i} \xi_i^{\mu} s_i\right) \qquad p(\boldsymbol{s}) = \frac{1}{Z} \exp\left(\sum_{\mu} \left[\sum_{i} \xi_i^{\mu} s_i\right]^2 - A \sum_{\mu} \left[\sum_{i} \xi_i^{\mu} s_i\right]^4 + \mathcal{O}(s^6)\right)$$

With non-linear response (not Gaussian), we can fit higher order statistics

The Restricted Boltzmann Machine

$$\mathcal{H}[\boldsymbol{s},\boldsymbol{\tau}] = -\sum_{i,a} s_i w_{ia} \tau_a - \sum_i a_i s_i - \sum_a b_a \tau_a$$

Discrete $s_i, \tau_a = \pm 1$ or $\{0,1\}$ Weights : $\{\boldsymbol{w}, \boldsymbol{a}, \boldsymbol{b}\}$

$$p(\boldsymbol{s}, \boldsymbol{\tau}) = \frac{1}{Z} \exp\left(-\mathcal{H}[\boldsymbol{s}, \boldsymbol{\tau}]\right)$$

The training is usually done by maximizing the likelihood

$$\mathcal{L} = \frac{1}{M} \sum_{m} \log \left(p(\boldsymbol{s}^{(m)}) \right) - \log Z$$
$$\frac{dw_{ia}}{dt} \sim \frac{\partial \mathcal{L}}{\partial w_{ia}} = \langle s_i \tau_a \rangle_{\text{data}} - \langle s_i \tau_a \rangle_{\mathcal{H}}$$

Curse of Monte Carlo

The Restricted Boltzmann Machine

Challenges :

- Practical training aspects : Monte Carlo problem
- Learning dynamics
- Landscape of the learned Machine

Mean-Field approach

In the small-weight regime – typically at the beginning of the learning -, we can try to describe the probability distribution on a set of uncoupled variables. → typically naive-MF, MF approximation etc

$$p_{\text{indep}}(\boldsymbol{s}, \boldsymbol{\tau}) = \prod_{i} p_{i}(s_{i}) \prod_{a}(\tau_{a}) \propto \prod_{i} e^{h_{i}s_{i}} \prod_{a} e^{h_{a}\tau_{a}}$$
$$\{h_{i}, h_{a}\} = \operatorname{argmin} D_{KL}(p_{RBM} || p_{\text{indep}})$$

$$m_{i} = \tanh\left(\sum_{a} w_{ia}m_{a} + a_{i}\right)$$
$$m_{a} = \tanh\left(\sum_{i} w_{ia}m_{i} + b_{a}\right)$$

1

Singular Values Eqs (in the linear regime)

 $egin{aligned} m{m}^{(vis)} &= m{W}m{m}^{(hid)} \ m{m}^{(hid)} &= m{W}^Tm{m}^{(vis)} \end{aligned}$

The paramagnetic fixed point is unstable for $\lambda_{max}\!=\!1$

Mean-Field approach

In the linear regime, the properties of the RBM is dominated by the spectral properties or ${\it W}$

Singular Values Eqs

(in the linear regime)

$$egin{aligned} m{m}^{(vis)} &= m{W}m{m}^{(hid)} \ m{m}^{(hid)} &= m{W}^Tm{m}^{(vis)} \end{aligned}$$



Consider the low-rank model matrix

$$w_{ia} = \sum_{\alpha=1}^{K} u_i^{\alpha} w_{\alpha} \bar{u}_a^{\alpha} + r_{ia}$$
$$r_{ia} \sim \mathcal{N}(0, \sigma)$$

 $m{r}, m{u}, \overline{m{u}}$: quenched average w_lpha are fixed



Linear learning dynamics

We can confirm this picture first by computing the gradient in the linear regime, in the SVD spa ce of the W matrix

$$\frac{dw_{\alpha}}{dt} = w_{\alpha} \left(\langle s_{\alpha}^2 \rangle_{\text{Data}} - 1 \right)$$

$$\bar{u}^{\alpha} \frac{d\boldsymbol{u}^{\beta}}{dt} = \Omega^{u}_{\alpha\beta} = (1 - \delta_{\alpha\beta}) \Big(\frac{w_{\beta} - w_{\alpha}}{w_{\alpha} + w_{\beta}} - \frac{w_{\beta} + w_{\alpha}}{w_{\alpha} - w_{\beta}} \Big) \langle s_{\alpha} s_{\beta} \rangle_{\text{Data}}$$

Empirical evidence on MNIST



We can solve the gradient equation in a simplified case

 \rightarrow we consider one Gaussian hidden node

 \rightarrow the dataset is generated by a Curie Weiss model in the low temperature regime

$$p_{\rm CW}(\boldsymbol{s}) = \frac{1}{Z} \exp\left(\beta \sum_{i < j} \xi_i \xi_j s_i s_j\right)$$
$$p_{\rm HF}(\boldsymbol{s}, \tau) = \frac{1}{Z} \exp\left(\sum_i s_i \tau w_i - \frac{\tau^2 N}{2}\right)$$

 $\boldsymbol{\xi}$ a preferred direction

The gradient for the weight matrix is given by

$$\frac{dw_i}{dt} = \langle s_i \tau \rangle_{\text{data}} - \langle s_i \tau \rangle_{\mathcal{H}}$$
$$= N^{-1} \sum_j \langle s_i s_j \rangle_{\text{data}} w_j - N^{-1} \sum_j \langle s_i s_j \rangle_{\mathcal{H}} w_j$$

The gradient for the weight matrix is given by

$$\frac{dw_i}{dt} = \langle s_i \tau \rangle_{\text{data}} - \langle s_i \tau \rangle_{\mathcal{H}}$$
$$= N^{-1} \sum_j \langle s_i s_j \rangle_{\text{data}} w_j - N^{-1} \sum_j \langle s_i s_j \rangle_{\mathcal{H}} w_j$$

The correlation of the dataset is given by

$$\langle s_i s_j \rangle_{\text{data}} = \xi_i \xi_j m^2$$
 where $m = \tanh(\beta m)$

The correlation of the RBM is given by

 $\langle s_i s_j \rangle_{\mathcal{H}} = \tanh(h^* w_i) \tanh(h^* w_j)$ where $h^* = \frac{1}{N} \sum_k w_k \tanh(h^* w_k)$

The correlation of the dataset is given by

$$\langle s_i s_j \rangle_{\text{data}} = \xi_i \xi_j m^2$$
 where $m = \tanh(\beta m)$

The correlation of the RBM is given by

$$\langle s_i s_j \rangle_{\mathcal{H}} = \tanh(h^* w_i) \tanh(h^* w_j)$$
 where $h^* = \frac{1}{N} \sum_k w_k \tanh(h^* w_k)$
 $\langle s_i s_j \rangle_{\mathcal{H}} \approx 0$ for small W

We can project the equations on

$$u_i = N^{-1/2} \xi_i$$
$$U_{\boldsymbol{\xi}} = \sum_i u_i w_i$$

 $\frac{dU_{\xi}}{dt} = U_{\xi}m^2 \Rightarrow U_{\xi}(t) = U_{\xi}(0)\exp(m^2t)$ Exponential growth in the direction of ξ

As the weights grow, we can for instance monitor the suceptibility of the model

$$\chi = \sum_{i,j} \xi_i \xi_j \langle s_i s_j \rangle_{\mathcal{H}} \approx \left(\xi_i s_i\right)^2 \frac{1}{N(1 - \sum_i w_i^2/N)}$$

It diverges as $\frac{1}{N}\sum_i w_i^2 \sim 1$

 \rightarrow signal of a phase transition, the magnetization departs from zero, the critical exponent associated to the sucesptibility is $\gamma\!=\!1$

At late learning time, we can show that \rightarrow the orthogonal directions to ξ are suppressed

 $\rightarrow w_i = w \xi_i \text{ and } w = \sqrt{\beta}$



We can also analyze the dynamics in the case of a binary-binary RBM

 $\alpha = \frac{N_h}{N}$



It is actually possible to study a problem with two correlated patterns

$$p(\mathbf{s}) = \frac{1}{Z} \exp\left(\frac{\beta}{2} \sum_{a} \left[\sum_{i} \xi_{i}^{a} s_{i}\right]^{2}\right)$$

$$\begin{aligned} \boldsymbol{\xi}^{1} &= \boldsymbol{\eta}^{1} + \boldsymbol{\eta}^{2} \\ \boldsymbol{\xi}^{2} &= \boldsymbol{\eta}^{1} - \boldsymbol{\eta}^{2} \\ \eta_{i}^{2} &= \begin{cases} \pm 1 \text{ if } 1 \leq i \leq N \frac{1+\kappa}{2} \\ 0 \text{ otherwise} \end{cases} \\ \boldsymbol{\xi}^{2} &= \boldsymbol{\eta}^{1} - \boldsymbol{\eta}^{2} \\ \eta_{i}^{2} &= \begin{cases} \pm 1 \text{ if } N \frac{1+\kappa}{2} + 1 \leq i \leq N \\ 0 \text{ otherwise} \end{cases} \end{aligned}$$

Theory of learning dynamics $\boldsymbol{\xi}^1 = \boldsymbol{\eta}^1 + \boldsymbol{\eta}^2$ with a simplified model of data $\boldsymbol{\xi}^2 = \boldsymbol{\eta}^1 - \boldsymbol{\eta}^2$

Phase diagram of such model :

$$m_1 = \frac{1+\kappa}{2} \tanh(\beta(m_1+m_2)) + \frac{1-\kappa}{2} \tanh(\beta(m_1-m_2))$$
$$m_2 = \frac{1+\kappa}{2} \tanh(\beta(m_1+m_2)) - \frac{1-\kappa}{2} \tanh(\beta(m_1-m_2))$$

At $T_1\!=\!1\!+\!\kappa$, magnetization along the direction $\pmb{\xi^1}$

 $m = \frac{1+\kappa}{2} \tanh\left(\beta 2m\right)$

At $T_2 \!=\! 1 \text{-} \kappa$, $m_1 \! \neq \! m_2$



We can decompose the correlation function of the dataset upon the SVD

 $\langle s_i s_j \rangle_{\mathcal{D}} = r^2 \eta_i^1 \eta_j^1 + p^2 \eta_i^2 \eta_j^2$

where
$$r = \tanh(\beta(m^+ + m^-))$$

 $p = \tanh(\beta(m^+ - m^-))$
 $m^+ = \max(m_1, m_2) \text{ and } m^- = \min(m_1, m_2)$

$$m_1 = \frac{1+\kappa}{2} \tanh(\beta(m_1+m_2)) + \frac{1-\kappa}{2} \tanh(\beta(m_1-m_2))$$
$$m_2 = \frac{1+\kappa}{2} \tanh(\beta(m_1+m_2)) - \frac{1-\kappa}{2} \tanh(\beta(m_1-m_2))$$

We can control the growth into each direction :

$$\boldsymbol{w}^{a}(t) = \frac{z^{a}}{\sqrt{\left(\frac{1+\kappa}{2}\right)}} e^{r^{2}\left(\frac{1+\kappa}{2}\right)t} \boldsymbol{\eta}^{1} + \frac{\tilde{z}^{a}}{\sqrt{\left(\frac{1-\kappa}{2}\right)}} e^{p^{2}\left(\frac{1-\kappa}{2}\right)t} \boldsymbol{\eta}^{2}$$

a = 1, 2





 h_1

 h_1

Numerical evidence

Are those transitions observed in this simple regime meanningful ? We the behavior of several training on various dataset :

- → MNIST
- \rightarrow genetic dataset
- → CelebA



MNIST



CelebA

28x28 pixels 10.000 samples 128x128 pixels 30.000 samples



Project Consortium

805 bases 4500 samples

Numerical evidence

What do we want to observe :

 \rightarrow phase transition as the eigenvalues pass a certain threshold

→ critical exponent $\chi = -\frac{\partial^2 \beta F}{\partial h^2} \sim_{T \to T_c} (T - T_c)^{-\gamma}$ (variance of the order parameter)

 \rightarrow relaxation time $au_{\exp} \sim_{T \rightarrow T_c} N^z$

→ hysteresis ? ... first order transition *in field*

Here, we will use binary {0,1} variables, for which the phase transition threshold is $\lambda = 4$

DNA dataset

Numerical evidence



MNIST dataset



epochs

CelebA dataset

Numerical evidence



How is that useful for ?

- Be carefull to the relaxation time (now you know)!
- Monitor the learning of the model
- Do these phenomena happen in other generative models (e.g. Diffusion)?
- You might want to use the « cascade of phase transition » to « understand » the model

Hierarchical carving

Now that we know that the landscape is shaped by a sequence of phase transitions, we can try to use them to explore what the RBM is learning.



Decelle, A., Rosset, L., & Seoane, B. PRE (2023)

We follow the maximum of the prob. Dist. using the Mean-Field equations



Lorenzo Rosset





Hierarchical carving

We can approximate the free energy using the Plefka expansion (small coupling)

$$\Gamma(\boldsymbol{m}^{(vis)}, \boldsymbol{m}^{(hid)}) \approx S(\boldsymbol{m}^{(vis)}, \boldsymbol{m}^{(hid)}) - \sum_{i} a_{i}m_{i} - \sum_{a} b_{a}m_{a}$$
$$-\sum_{ia} \left[w_{ia}m_{i}m_{a} + \frac{w_{ia}^{2}}{2}(m_{i} - m_{i}^{2})(m_{a} - m_{a}^{2}) \right]$$

Self-consistent eqs.
$$\begin{pmatrix}
m_i = \operatorname{sigm}(a_i + \sum_a w_{ia}m_a - \sum_a w_{ia}^2 \left(m_i - \frac{1}{2}\right) (m_a - m_a^2)) \\
m_a = \operatorname{sigm}(b_a + \sum_i w_{ia}m_i - \sum_i w_{ia}^2 \left(m_a - \frac{1}{2}\right) (m_i - m_i^2))
\end{cases}$$

Gabrié et al, Neurips 2015

1

- 1

 $sigm(x) = (1 + exp(-x))^{-1}$

Example on the genetic dataset

- <u>5008 sequences</u> of mutated or not (0/1) genes (samples)
- <u>805 genes</u> (variables)



Tree reconstruction of the minima

Learning Trajectory

Building a hierarchical tree from it !

Younger RBMs

: fixed points
 : initial conditions

(Old)



On MNIST

7
8
9

Toward the center: older and older machines **The leafs**: dataset





On DNA dataset





Conclusion

- RBMs undergoe phase transition at the beginning of the learning
- We can associate mean-field critical exponents to this transition
- Concrete effect : the relaxation time diverges
 → strong constraints on the Monte Carlo estimation
- Possible application : Hierarchical shattering of the landscape as the learning goes