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

Paris-Saclay

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

$$
p(\boldsymbol{\theta} \vert \mathcal{D}) = \tfrac{p(\mathcal{D} \vert \boldsymbol{\theta}) p(\boldsymbol{\theta})}{Z(\mathcal{D})}
$$

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

- → 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

- Supervised Learning
- Unsupervised Learning

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

$$
\{x_m\}_{m=1,\ldots,M} \quad \{y_m\}_m
$$
\nExample of
\n
$$
x = \text{Example\n
$$
y = \text{"cats"}
$$
\nExpression

\n
$$
y = \text{"cats"}
$$
\nregression
$$

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
- Unsupervised Learning

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

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 mixture model: distribution 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

Hopfield model : 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

The Restricted Boltzmann Machine : generative model \rightarrow 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 $s_i\!=\!\pm 1$

$$
\mathcal{H} = -\frac{1}{N} \sum_{i} J_{ij} s_i s_j = -\frac{1}{2N} \sum_{\mu} \left(\sum_{i} s_i \xi_i^{\mu} \right)^2
$$

$$
J_{ij} = \sum_{\mu} \xi_i^{\mu} \xi_j^{\mu}
$$

$$
\xi_i^{\mu} = \pm 1 \text{ with } p = 1/2 \text{ and } \mu = 1, ..., P = \alpha N
$$

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

Order parameters \overline{a}

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

$$
m = \frac{1}{N} \sum_{i} \xi_i^{\mu} \langle s_i \rangle
$$

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

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

$$
p(\boldsymbol{s}) = \frac{1}{Z} \exp(-\beta \mathcal{H}[\boldsymbol{s}])
$$

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

Credit to Barra et al. 2018

From Hopfield to Bipartite architecture

 $\mathcal{H}_{\rm RBM}[{\bm{s}}, {\bm{\tau}}] = -\sum_{i\mu}s_i w_{i\mu}\tau_\mu$

<u>linear response from the hidden layer</u> credit to Barra et al. 2018

From Hopfield to Bipartite architecture

 $\mathcal{H}_{\rm RBM}[{\bm{s}}, {\bm{\tau}}] = -\sum_{i\mu}s_i w_{i\mu}\tau_\mu,$

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

$$
p(s_i|\boldsymbol{\tau}) = \tanh\left(\sum_{\mu} \xi_i^{\mu} \tau_{\mu}\right)
$$

Distribution on the spins:

$$
p(\tau_{\mu}|\boldsymbol{s}) = \tanh\left(\sum_{i} \xi_i^{\mu} s_i\right)
$$

$$
p(\boldsymbol{s}) = \frac{1}{Z} \exp\left(\sum_{\mu} \left[\sum_{i} \xi_i^{\mu} s_i\right]^2 - A \sum_{\mu} \left[\sum_{i} \xi_i^{\mu} s_i\right]^4 + \mathcal{O}(s^6)\right)
$$

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

The Restricted Boltzmann Machine

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

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

Contract Contract Street

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

The training is usually done by maximizing the likelihood

$$
\mathcal{L} = \frac{1}{M} \sum_{m} \log (p(\mathbf{s}^{(m)})) - \log Z
$$

$$
\frac{dw_{ia}}{dt} \sim \frac{\partial \mathcal{L}}{\partial w_{ia}} = \langle s_i \tau_a \rangle_{\text{data}} - \langle s_i \tau_a \rangle_{\mathcal{H}}
$$

$$
W_{11}
$$
\n
$$
W_{12}
$$
\n
$$
W_{13}
$$
\n
$$
W_{N_hN_v}
$$
\n
$$
W_{N_hN_v}
$$
\n
$$
W_{N_hN_v}
$$
\n
$$
W_{N_hN_v}
$$
\n
$$
V_{13}
$$
\n
$$
V_{14}
$$
\n
$$
V_{15}
$$
\n
$$
V_{16}
$$
\n
$$
V_{17}
$$
\n
$$
V_{18}
$$

 $\overline{}$

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. \rightarrow typically naive-MF, MF approximation etc

 $(1 \cdot 1)$

$$
p_{\text{indep}}(s, \tau) = \prod_{i} p_i(s_i) \prod_a(\tau_a) \propto \prod_{i} e^{h_i s_i} \prod_a e^{h_a \tau_a}
$$

$$
\{h_i, h_a\} = \operatorname{argmin} D_{KL}(p_{RBM} || p_{\text{indep}})
$$

$$
m_i = \tanh\left(\sum_a w_{ia} m_a + a_i\right)
$$

$$
m_a = \tanh\left(\sum_i w_{ia} m_i + b_a\right)
$$

 $\overline{ }$

Singular Values Eqs (in the linear regime)

$$
\boldsymbol{m}^{(vis)} = \boldsymbol{W}\boldsymbol{m}^{(hid)}\\ \boldsymbol{m}^{(hid)} = \boldsymbol{W}^T \boldsymbol{m}^{(vis)}
$$

 $\sqrt{2}$ $\sqrt{2}$

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

Mean-Field approach

In the linear regime, the properties of the RBM is dominated by the spectral properties or W

Singular Values Eqs

(in the linear regime)

$$
\begin{aligned} \boldsymbol{m}^{(vis)} &= \boldsymbol{W}\boldsymbol{m}^{(hid)} \\ \boldsymbol{m}^{(hid)} &= \boldsymbol{W}^T\boldsymbol{m}^{(vis)} \end{aligned}
$$

Consider the low-rank model matrix

$$
w_{ia} = \sum_{\alpha=1}^{K} u_i^{\alpha} w_{\alpha} \bar{u}_a^{\alpha} + r_{ia}
$$

$$
r_{ia} \sim \mathcal{N}(0, \sigma)
$$

 r,u,\overline{u} : quenched average w_{α} 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

$$
\frac{d w_\alpha}{dt} = w_\alpha \Bigl(\langle s_\alpha^2 \rangle_{\text{Data}} - 1 \Bigr)
$$

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

Empirical evidence on MNIST

We can solve the gradient equation in a simplified case

→ we consider one Gaussian hidden node

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

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

ξ 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

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

$$
\langle s_i s_j \rangle_{\mathcal{H}} \approx 0 \quad \text{for small } \mathbf{W}
$$

$$
\frac{dw_i}{dt} = \frac{1}{N} \xi_i \sum_j \xi_j w_j m^2
$$

We can project the equations on

$$
u_i = N^{-1/2}\xi_i
$$

$$
U_{\xi} = \sum_i u_i w_i
$$

 $\frac{dU_{\xi}}{dt} = U_{\xi} m^2 \Rightarrow U_{\xi}(t) = U_{\xi}(0) \exp(m^2 t)$ 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

 $\rightarrow w_i \!=\! w\, \xi_i$ 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

$$
p(\boldsymbol{s}) = \frac{1}{Z} \exp \left(\frac{\beta}{2} \sum_{a} \left[\sum_{i} \xi_i^a s_i \right]^2 \right)
$$

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

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

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

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 $\pmb{\xi}^{\!\text{1}}$

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

At $T_2 = 1-\kappa$, $m_1 \neq m_2$

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

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

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

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

We can control the growth into each direction :

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

 $a = 1, 2$

Numerical evidence

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

- \rightarrow MNIST
- \rightarrow genetic dataset
- \rightarrow CelebA

28x28 pixels 10.000 samples

128x128 pixels 30.000 samples

805 bases 4500 samples

Numerical evidence

What do we want to observe :

 \rightarrow phase transition as the eigenvalues pass a certain threshold

 \rightarrow critical exponent (variance of the order parameter)

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

→ 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

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

Gabrié et al, Neurips 2015

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

Example on the genetic dataset

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

Tree reconstruction of the minima

Learning Trajectory

Building a hierarchical tree from it !

On MNIST

 2 3 $\sqrt{4}$ ◯ 5 6 \triangleright 7 $\overline{)8}$ \bigcirc 9

Toward the center: older and older machines The leafs: dataset $\overline{0}$

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 \rightarrow strong constraints on the Monte Carlo estimation
- Possible application: Hierarchical shattering of the landscape as the learning goes