Restricted Boltzmann Machines

On Restricted Boltzmann Machines (RBMs) with non-linear type architectures and compositional phase.

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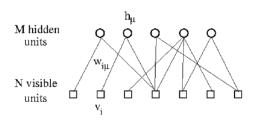
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- ► RBMs are unsupervised algoritms: learning features from data without any a priori knowledge
- RBM structure:

$$E[\boldsymbol{v}, \boldsymbol{h}] = -\sum_{i=1}^{N} \sum_{\mu=1}^{M} w_{i\mu} v_i h_{\mu} - \sum_{i=1}^{N} \mathcal{U}_i(v_i) + \sum_{\mu=1}^{M} \mathcal{U}_{\mu}(h_{\mu})$$
 (1)



J.Tubiana, R.Monasson (2017)

- ightharpoonup Change hidden units potential (\mathcal{U}_{μ}) affects performance
- ▶ The dynamics of the network (Metropolis) gives Boltzmann distribution at equilibrium: $P(v, h) = \frac{1}{Z}e^{-E(v,h)/T}$
- ▶ Because of "Conditional independence property": $P(\boldsymbol{h}|\boldsymbol{v}) = \prod_{\mu} P(h_{\mu}|\boldsymbol{v})$ we can get the probability of a given unit to be active:

$$P(h_{\mu}|\boldsymbol{v}) = \frac{e^{h_{\mu}I_{\mu} - \mathcal{U}_{\mu}(h_{\mu})}}{Z(\boldsymbol{h}|\boldsymbol{v})}$$

where $I_{\mu} = \sum_{i} w_{i\mu} v_{i}$

Definition

 $\phi_\mu:=$ activation function for $h_\mu:$ most probable value h_μ^* of the hidden unit μ given the configuration v

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► The most probable value is linked to the Energy-based behaviour of the RBM

$$\begin{split} h_{\mu}^* &= \phi_{\mu}(I_{\mu}) = \operatorname*{argmax}_{h_{\mu}} P(h_{\mu}|\boldsymbol{v}) \\ \phi_{\mu}(I_{\mu}) &= \operatorname*{argmax}_{h_{\mu}} \frac{P(h_{\mu}, \boldsymbol{v})}{P(\boldsymbol{v})} = \operatorname*{argmax}_{h_{\mu}} \frac{e^{-E(\boldsymbol{v}, \boldsymbol{h})}}{Z} \\ &\equiv \operatorname*{argmin}_{h_{\mu}} E(\boldsymbol{h}, \boldsymbol{v}) \end{split}$$

 \blacktriangleright Most probable hidden unit state h_μ^* is given by minimization of the Energy

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Most probable hidden unit state h_{μ}^{*} is given by minimization of the Energy

$$\frac{\partial E(\boldsymbol{h}, \boldsymbol{v})}{\partial h_{\mu}} = \sum_{i,\nu} \left[-w_{i\mu}v_{i} + \frac{\partial \mathcal{U}_{\nu}}{\partial h_{\mu}} \right] \delta_{\mu,\nu} \bigg|_{h_{\mu}^{*}} = 0$$

$$-w_{i\mu}v_{i} + \frac{\partial \mathcal{U}_{\mu}}{\partial h_{\mu}} \left(h_{\mu}^{*} \right) = 0$$

$$\implies h_{\mu}^{*} = \left(\frac{\partial \mathcal{U}_{\mu}}{\partial h_{\mu}} \right)^{-1} (I_{\mu})$$

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Consequences in the Gibbs sampling procedure of the gradient descent method:

- 1. Starting from initial $oldsymbol{v}$
- 2. $I_{\mu} \rightarrow P(h_{\mu}|\boldsymbol{v}) \quad \forall_{\mu=1...M} \rightarrow \boldsymbol{h^*}$
- 3. $I_i \to P(v_i|\boldsymbol{h}) \quad \forall_{i=1...N} \to \boldsymbol{v}^*$

Learning algorithm:

$$\frac{\partial \mathcal{L}}{\partial w_{i,\mu}} = <\!\! v_i h_\mu \!\!>_{data} - <\!\! v_i h_\mu \!\!>_{model}$$

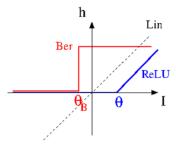
where \mathcal{L} is the log likelihood

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Different activation functions:

Property	Bernoulli	Gaussian	Rectified Linear
Domain	$\mathcal{X} \in \{0,1\}$	$\mathcal{X} \in \mathbb{R}$	$\mathcal{X} \in [0, +\infty)$
Potential	$\mathcal{U} = -g\mathcal{X}$	$\mathcal{U} = rac{1}{2}\mathcal{X}^2$	$\mathcal{U} = \frac{1}{2}\mathcal{X}^2 + \theta\mathcal{X}$
Activation function	$\Phi = \Theta(x - g)$	$\Phi = x$	$\Phi = \max\{0, x - \theta\}$

Table 1: Activation functions

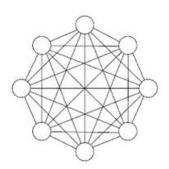


J.Tubiana, R.Monasson (2017)

Hopfield model

The RBMs framework can describe many different kind of interactions between visible units, using its interanl representation (h). An example is the Hopfield network.

$$E[v] = -\sum_{i=1}^{n} \sum_{j=1}^{n} v_i J_{ij} v_j - \sum_{i=1}^{n} a_i(v_i)$$



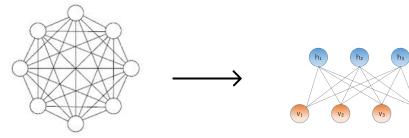
Hopfield network

Hopfield network

The Hubbard-Stratonovich (HS) transformation can be performed to link the Hopfield network to its RBM counterpart, rewriting $J_{ij} = \sum_{\mu} w_{i\mu} w_{j\mu}$:

$$\mathsf{P}(\boldsymbol{v}) = \frac{1}{Z} e^{\sum_{ij\mu} v_i w_{i\mu} w_{j\mu} v_j + \sum_{i=1}^N a_i(v_i)} \to \frac{1}{Z} e^{\sum_{i=1}^N a_i(v_i)} \prod_{\mu} \int_{\mu} e^{\sum_{\mu} h_{\mu}^2 + \sum_{i\mu} v_i w_{i\mu} h_{\mu}}$$

$$E[{\pmb v}] = -\sum_{i=1} \sum_j v_i J_{ij} v_j - \sum_i a_i(v_i) \to E[{\pmb v}, {\pmb h}] = -\sum_i a_i(v_i) + \frac{1}{2} \sum_\mu h_\mu^2 + \sum_{i\mu} w_{i\mu} v_i h_\mu$$



Hopfield network

RBM network

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Hopfield network

The above argument can be reversed starting from a general form of RBM energy (1).

$$P(\boldsymbol{v}) = \int \mathrm{d}\boldsymbol{h} P(\boldsymbol{v},\boldsymbol{h}) = \int \mathrm{d}\boldsymbol{h} \, \frac{1}{\mathcal{Z}} e^{-E(\boldsymbol{v},\boldsymbol{h})} \text{ and } P(\boldsymbol{v}) = \frac{1}{\mathcal{Z}} e^{-E(\boldsymbol{v})}$$

$$E(\boldsymbol{v}) = -\log \int d\boldsymbol{h} e^{-E(\boldsymbol{v},\boldsymbol{h})}$$

$$= -\sum_{i} a_{i}(v_{i}) - \sum_{\mu} \log \int dh_{\mu} e^{\frac{1}{2}\sum_{\mu} h_{\mu}^{2} + \sum_{i\mu} w_{i\mu} v_{i} h_{\mu}}$$

 Using the cumulant generating function and the hidden units distribution

$$K_{\mu} = \log \int dh_{\mu} q_{\mu}(h_{\mu}) e^{th_{\mu}}$$
 with
$$= \sum_{n} k_{\mu}^{(n)} \frac{t^{n}}{n!}$$

$$q_{\mu}(h_{\mu}) = \frac{1}{\mathcal{Z}} e^{\mathcal{U}_{\mu}(h_{\mu})}$$

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<u>Limits of Hopfield model</u>

Since Hopfield networks realize only a pair interaction between visible units it is easy to understand its limit in the learning procedure. Here is results of an argument based on a statistical mechanics approach (Amit, Gutfreund and Sompolinsky)

Hopfield Hamiltonian:

$$H(\mathbf{v}) = -\frac{1}{2} \sum_{ij, i \neq j} \frac{1}{N} \sum_{\mu} \xi_{i}^{\mu} \xi_{j}^{\mu} v_{i} v_{j}$$

 $H(\boldsymbol{v}) = -\frac{1}{2} \sum_{ij,i \neq j} \frac{1}{N} \sum_{\mu} \xi_i^{\mu} \xi_j^{\mu} v_i v_j \begin{cases} f = \frac{1}{2} \boldsymbol{m}^2 - \frac{1}{\beta} \langle \log[2\cosh(\beta \, \boldsymbol{m} \cdot \boldsymbol{\xi_i})] \rangle \\ \boldsymbol{m} = \langle \boldsymbol{\xi_i} \tanh(\beta \, \boldsymbol{m} \cdot \boldsymbol{\xi_i})] \rangle \end{cases}$

Overlap or magnetization:

$$m_{\mu} = \frac{1}{N} \sum_{i} v_{i} \xi_{i}^{\mu}$$

It is the case of a small number of patterns: $\alpha = \frac{M}{N} << 1$

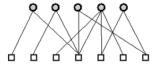
Distribution of i.i.d. weights $\xi_i^{\mu} = \begin{cases} +1 & \text{with prob } \frac{1}{2} \\ -1 & \text{with prob } \frac{1}{2} \end{cases}$

Hopfield phase transition

Two different solutions

Above $T \sim 1$

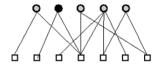
$$\begin{cases} f = -T \log(2) \\ \boldsymbol{m} = 0 \end{cases}$$



Spin-glass phase

Around $T\sim 0$

$$\begin{cases} f = -\frac{1}{2} \boldsymbol{m}^2 \\ \boldsymbol{m} = \left\langle \boldsymbol{\xi_i} \operatorname{sgn}(\boldsymbol{m} \cdot \boldsymbol{\xi_i}) \right\rangle \end{cases}$$



Ferromagnetic phase

In particular m^2 is bounded: $m^2 \le 1$ and the minimal states are of the kind m = (1,0,0,...,0)

Many patterns

Free energy $f=-\frac{1}{N\beta}{<}logTr(e^{-\beta H}){>}$ with α finite leads to different saddle point equations: f

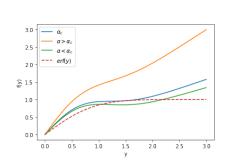
$$\begin{cases}
\mathbf{m} = \langle \xi_i \tanh[\beta(\alpha r)^{1/2} z + \mathbf{m} \cdot \boldsymbol{\xi_i}] \rangle \\
q = \langle \tanh^2[\beta(\alpha r)^{1/2} z + \mathbf{m} \cdot \boldsymbol{\xi_i}] \rangle \\
r = q[1 - \beta(1 - q)]^{-2}
\end{cases} \qquad \mathsf{T} \to 0$$

$$\begin{cases}
m = \mathsf{erf}\left(\frac{m}{\sqrt{2\alpha r}}\right) \\
q = 1 \\
r = (1 - C)^{-2}
\end{cases}$$

$$C = \sqrt{\frac{2}{\pi \alpha r}} e^{-\frac{m^2}{2\alpha r}}$$

Using the change of variables:

- ► $y = \frac{m}{\sqrt{2\alpha r}}$ the magnetization equation gives :
- $y(\sqrt{2\alpha} + \frac{2}{\sqrt{\pi}}e^{-y^2}) = \operatorname{erf}(y)$



Critical capacity $\alpha_c \approx 0.138$

Connection with Gaussian RBM

- ► The Hopfield network can be recasted in a RBM with a Gaussian hidden layer: $\mathcal{U}(h) = \frac{h^2}{2}$, with zero visible strength: g = 0
- ► The pattern retrieval can be reinterpreted in an RBM optics
- ightharpoonup Consider Bernoulli visible units $v_i \in \{-1,1\}$ with step activation funcion (Tab.1)
- $lackbrack I_{\mu}(oldsymbol{v}) = \sqrt{N} m_{\mu}(oldsymbol{v})$ then the most probable value h_{μ}^{*} is $h_{\mu}^{*} = I_{\mu}$

RBMs

Pattern retrival

- Supose v is a (single) memory pattern: $v=\xi_1$
- $h_1^* = I_1 = \sqrt{N} m_1(\xi_1) = \sqrt{N}$
- $\blacktriangleright \ h_{\mu}^* = \sqrt{N} \sum_i \frac{\xi_{i1} \xi_{i\mu}}{N} \bigg|_{\mu \neq 1} \sim \mathcal{N}(0, 1)$
- ► From Gibbs sampling:

$$\mathbf{v} \to \mathbf{h} = (\sqrt{N}, h_2^*, ...)$$

 $\mathbf{h} \to v_i = \Theta(\xi_{i1} + \sqrt{N} \sum_{\mu \neq 1}^{M} \xi_{i\mu} h_{\mu}^*)$

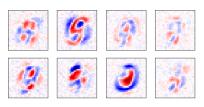
▶ In order to retrieve the initial pattern the second contribution needs to be less than 1. This is obtained by $\frac{M}{N} < 1$. In the limit $N \to \infty$ we need e.g. M to be finite

Choosing a non linear transfer function such as ReLU is a simple way to suppress undesired inputs.

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Simulations on MNIST

A simulation of an RBM-Gaussian machine with $\alpha \approx 0.26$ shows that weights have a "chaotic" behaviour.



RBM-Gaussian weights

Many interactions with similar strenght

Many weights compete among each other and the resulting generative power of the machine decrease











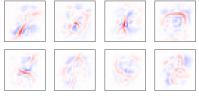




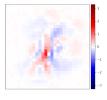


ReLU-RBM simulation on MNIST

The result of a ReLU-RBM with the same number of hidden units substantially different



RBM-ReLU weights



Sparse connection with few stronger

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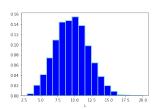
Different combination of the (stronger) learned features are combined to produce different variants of the same digits. Manyof those are not contained in the training set

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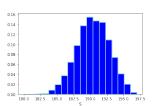
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Strongly activated hidden units

In each generated handwritten digit image lots of hidden units are silent, while the remaining has largely varying activations, some weak and few very strong.



Strongly activated hidden units (L)



Silent hidden units (S)

 ${\cal L}$ can be estimated by the participation ratio:

$$\hat{L} = [(\sum_{\mu} h_{\mu})^a)^2/(\sum_{\mu} h_{\mu}^{2a})] = PR_a(h)$$

The value of a is set to 3.

Starting from a typical configuration h:

$$h_{\mu} = \begin{cases} m\sqrt{N} & \text{if} \quad 1 \le \mu \le L \\ \sqrt{r}x_{\mu} & \text{if} \quad L + 1 \le \mu \le M \end{cases}$$

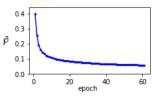
$$\begin{split} PR_3(h) &\sim \frac{(Lm^3N^{3/2} + (N-L)r^{3/2})^2}{Lm^6N^3 + (N-L)r^3} \\ &= L \times \frac{(1 + \frac{(N-L)}{N^{3/2}} \frac{r^{3/2}}{Lm^3})^2}{1 + \frac{(N-L)}{N^3} \frac{r^3}{Lm^6}} \xrightarrow{N \to \infty} L \end{split}$$

Compositional phase

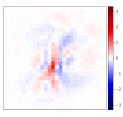
The machine finish the training with more than one strongly activated hidden unit

Weight sparsity

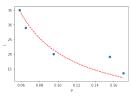
► After training the machine reach a low degree of sparsity



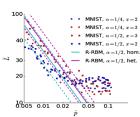
Weight sparsity: $\,\hat{p}=\frac{1}{MN}\sum_{\mu}[(\sum_{i}w_{i\mu}^{2})/(\sum_{i}w_{i\mu}^{4})]\,$



▶ Different RBMs has reach different sparsity values. This affects also *L*



 $L \sim \ell^*/p$



J.Tubiana, R.Monasson (2017)

Replica theory

Studies related to Random RBMs (R-RBMs) support the observations.

- ► Assumption:
 - system state $(E1, E2, ..., E_N)$
 - system distribution $\mu_B(j) = \frac{1}{Z}e^{-\beta E_j}$
 - E_i i.i.d. $\sim e.g. \mathcal{N}(0, \sigma^2)$
- ▶ The Replica trick allows to obtain easily $\mathbb{E} log Z \sim f$
- Instead of computing $\mathbb{E} log Z$ it results easyer computing $\mathbb{E} Z^n$
- $\blacktriangleright \mathbb{E} \log Z = \lim_{n \to 0} \frac{\mathbb{E}(Z^n) 1}{n}$

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Replica theory

 R-RBM ensamble are characterized by random patterns

$$w_{i\mu} = \begin{cases} +1/\sqrt{N} & \frac{p_i}{2} \\ -1/\sqrt{N} & \frac{p_i}{2} \end{cases} \qquad p_i \in [0,1]$$

$$0 \quad 1 - p_i$$

Energy of the general bipartite network

$$E(\boldsymbol{v}, \boldsymbol{h}) = -\sum_{i=1}^{N} \sum_{\mu=1}^{M} w_{i\mu} v_{i} h_{\mu} + \sum_{i=1}^{N} \mathcal{U}_{v}(v_{i}) + \sum_{\mu=1}^{M} \mathcal{U}_{h}(h_{\mu})$$

Partition function

$$Z = = \sum_{\{\boldsymbol{v}\}} \sum_{\{\boldsymbol{h}\}} e^{-\beta E(\boldsymbol{v}, \boldsymbol{h})}$$

► Replica partion function

$$Z^{n} = \int (\prod_{i,a} dv_{i,a}) \times$$

$$\times \int (\prod_{\mu,a} dh_{\mu,a}) e^{-\beta E(\boldsymbol{v}_{a},\boldsymbol{h}_{a})}$$

Towards free energy

▶ Simulations allow to make an ansatz for the hidden units: fixing e.g. the first L to be the strongly activated ones $h_1^a = h_2^a = ... = h_I^a = m\sqrt{N}$

$$Z^{n} = \int (\prod_{i,a} dv_{i,a}) \int (\prod_{\mu,a} dh_{\mu,a}) \exp\left[-\sum_{a} \beta L \mathcal{U}_{h}(m\sqrt{N}) - \sum_{a,\mu>L} \beta \mathcal{U}_{h}(h_{\mu}^{a})\right]$$
$$-\beta m\sqrt{N} L \sum_{i,\mu=1} \int_{L} w_{i\mu} \sum_{a} v_{i}^{a} - \beta \sum_{i,\mu>L} w_{i\mu} \sum_{a} v_{i}^{a} h_{\mu}^{a}$$

▶ The average of Z^n on the last term brings to a quartic interaction term $\sim v_i^a\,v_i^b\,h_\mu^a\,h_\mu^b$. The decoupling is done by the HS transformation that produce new fields

$$\begin{split} \bar{Z}^n &= \prod_{a \leq b} \frac{\mathrm{d}\bar{q}^{ab} \mathrm{d}q^{ab}}{2N\beta} \exp \left[-\beta \, N \sum_{a \leq b} \bar{q}^{ab} q^{ab} - \beta \, n \, L \, \mathcal{U}_h(m\sqrt{N}) \right] \times \\ &\times \prod_i \prod_a \int \mathrm{d}v_i^a \exp \left[-\beta \sum_a \mathcal{U}_v(v_i^a) + \beta \sum_{a \leq b} \bar{q}^{ab} v_i^a v_i^b \frac{p_i}{p} + \beta \, m \left(\sum_{\mu}^L \sqrt{N} w_{i\mu} \right) \left(\sum_a v_i^a \right) \right] \times \\ &\times \left(\prod_a \int \mathrm{d}h^a \exp \left[-\beta \sum_a \mathcal{U}_h(h^a) + \frac{\beta^2 p}{2} \sum_{a \leq b} q^{ab} h^a h^b \frac{p_i}{p} \right] \right)^{\alpha \, N - L} \end{split}$$

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Towards free energy

- ▶ Functional form of $\bar{Z}^n = \int da \, db, ... e^{-\beta F(a,b,...)}$
- ▶ Saddle-point approximation $\bar{Z}^n \approx \exp(-\beta F(a,b,...)\big|_{a^*,b^*,...}$ $(a^*,b^*,...)$ are the saddle point value of F
- $ightharpoonup |\bar{Z}^n \approx 1 \beta F(a, b, ...)|_{a^*, b^*, ...}$
- ► Free energy:

$$f = \frac{L \, m^2}{2} + \frac{\alpha}{2} (r \, C + B \, q) + \alpha \frac{1}{N} \sum_{i} \langle \int Dz \, \min_{v} \left[\mathcal{U}_{v}(v) - (m \, W + z \sqrt{\alpha \pi r})v - \frac{\alpha}{2} B \frac{p_{i}}{p} v^{2} \right] \rangle_{W} + \alpha \int Dz \, \min_{h} \left[\mathcal{U}_{h}(h) - \frac{C}{2} h^{2} - z \sqrt{\alpha p \, r} \right]$$

where

Replica symmetric ansatz

$$\begin{cases} W = \sqrt{N} \sum_{\mu} w_{i\mu} \\ p = \sum_{i} \frac{p_{i}}{N} \end{cases} \qquad \begin{cases} q^{ab} = q + \delta_{ab} \frac{C}{p\beta} \\ \bar{q}^{ab} = \frac{\alpha\beta p}{2} \left[2r(1 - \delta_{ab}) + \delta_{ab}(r + \frac{B}{p\beta}) \right] \end{cases}$$

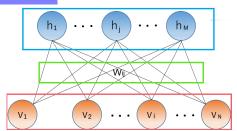
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Free energy and RBM structure

$$f = \frac{L m^2}{2} + \alpha \int Dz \min_{h} \left[\mathcal{U}_h(h) - \frac{C}{2} h^2 - \right]$$

$$z\sqrt{\alpha p \, r}$$

$$+\frac{\alpha}{2}(r\,C+B\,q)$$



$$+\alpha \frac{1}{N} \sum_{i} \langle \int Dz \min_{v} \left[\mathcal{U}_{v}(v) - (mW) + z\sqrt{\alpha \pi r} \right] v - \frac{\alpha}{2} B \frac{p_{i}}{p} v^{2} \rangle_{W}$$

RBMs

Parameter interpretation

The saddle point equations (e.g. $\frac{\partial (-\beta F/N)}{\partial q^{ab}} = 0$) give insights about the interpretation of the saddle point parameters

$$\begin{split} q &= \overline{\frac{1}{N} \sum_{i} \frac{p_{i}}{p} \left\langle v_{i} \right\rangle^{2}} \approx_{\beta \to \infty} \overline{\frac{1}{N} \sum_{i} \frac{p_{i}}{p} \left\langle v_{i} \right\rangle} \\ r &= \overline{\frac{1}{M - L} \sum_{\mu > L} \left\langle h_{\mu} \right\rangle^{2}} \end{split} \qquad \begin{aligned} C &= \lim_{\beta \to \infty} \overline{\frac{\beta p}{N} \sum_{i} \frac{p_{i}}{p} \left\langle v_{i} \right\rangle \left(1 - \left\langle v_{i} \right\rangle\right)} \\ B &= \lim_{\beta \to \infty} \overline{\frac{\beta p}{M - L} \sum_{\mu > L} \left\langle h_{\mu}^{2} \right\rangle - \left\langle h_{\mu} \right\rangle^{2}} \end{aligned}$$

J. Tubiana, R. Monasson (2017)

J.Tubiana, R.Monasson (2017)

lackbox(q,r,C,B) are respectively the (weighted) mean activity in the visible layer, the square average activation of the weakly activated hidden units, the rescaled variance of the visible and hidden units.

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Homogeneus free energy

- ▶ Solution for the homogeneus case $(p_i \equiv p)$, Bernoulli visible units with constant strenght $(g_i \equiv g)$ and ReLU hidden units:
- $f_{GS}(L, m, r, B, q, C) = \frac{L m^2}{2} + \frac{\alpha}{2} (r C + B q) \sqrt{\alpha p r} \langle H^{(1)} \Big(\left[\frac{g + m W + \alpha B/2}{\sqrt{\alpha p r}} \right] \Big) \rangle_W + \frac{\alpha p q}{2(1 C)} H^{(2)} \Big(\frac{\theta}{\sqrt{pq}} \Big)$

where $H^{(k)}(x) = \int_{x}^{\infty} Dz(z-x)^{k}$ and Dz is the Gaussian measure

► Saddle point equations:

$$\begin{split} m &= \frac{1}{L} \langle WH^{(0)} \Big(- \left[\frac{g + mW + \alpha B/2}{\sqrt{\alpha p r}} \right] \Big) \rangle_W & r &= \frac{pq}{(1 - C)^2} H^{(2)} \Big(\frac{\theta}{\sqrt{pq}} \Big) \\ q &= \langle H^{(0)} \Big(- \left[\frac{g + mW + \alpha B/2}{\sqrt{\alpha p r}} \right] \Big) \rangle_W & B &= \frac{p}{(1 - C)} H^{(0)} \Big(\frac{\theta}{\sqrt{pq}} \Big) \\ C &= \frac{\sqrt{p}}{\sqrt{2 \pi c \sigma}} \langle e^{-\frac{1}{2} \frac{-(g + mW + \alpha B/2)^2}{\alpha p r}} \rangle_W \end{split}$$

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Homogeneus free energy

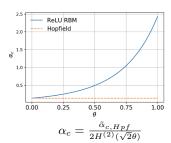
▶ Using Feynman integration techniques the energy and the equations can be also recast in a different form:

$$\begin{split} f_{GS}(L,m,r,B,q,C) &= \frac{L\,m^2}{2} + \frac{\alpha}{2}(r\,C+B\,q) - \sqrt{\alpha p\,r} \bigg\langle \frac{1}{2}e^{-\frac{1}{2}(\frac{(g+m\,W+\alpha B/2)^2}{\alpha\,p\,r}} + \\ &+ \frac{1}{2}\bigg(\frac{g+m\,W+\alpha B/2}{\sqrt{\alpha p\,r}}\bigg) \bigg(1 + \mathrm{erf}\Big(\frac{g+m\,W+\alpha B/2}{\sqrt{2\alpha p\,r}}\Big)\bigg)\bigg\rangle_W - \frac{\alpha pq}{2(1-C)}\,\frac{1}{2}e^{-\frac{1}{2}\frac{\theta^2}{pq}}\bigg[-\sqrt{\frac{2}{\pi}}\frac{\theta}{\sqrt{pq}} + \\ &+ e^{\frac{1}{2}\frac{\theta^2}{pq}}\Big(1 + \frac{\theta^2}{pq}\Big) \bigg(1 + \mathrm{erf}\Big(\frac{\theta}{\sqrt{2pq}}\Big)\bigg)\bigg] \\ &m = \frac{1}{L}\bigg\langle W\frac{1}{2}\bigg(1 + \mathrm{erf}\Big(\frac{g+m\,W+\alpha B/2}{\sqrt{2\alpha p\,r}}\Big)\bigg)\bigg\rangle_W \qquad r = \frac{pq}{(1-C)^2}\frac{1}{2}e^{-\frac{1}{2}\frac{\theta^2}{pq}}\bigg[-\sqrt{\frac{2}{\pi}}\frac{\theta}{\sqrt{pq}} + \\ &q = \bigg\langle \frac{1}{2}\bigg(1 + \mathrm{erf}\Big(\frac{g+m\,W+\alpha B/2}{\sqrt{2\alpha p\,r}}\Big)\bigg)\bigg\rangle_W \qquad + e^{\frac{1}{2}\frac{\theta^2}{pq}}\Big(1 + \frac{\theta^2}{pq}\Big)\bigg(1 + \mathrm{erf}\Big(\frac{\theta}{\sqrt{2pq}}\Big)\bigg)\bigg] \\ &C = \frac{\sqrt{p}}{\sqrt{2\pi\alpha r}}\langle e^{-\frac{1}{2}\frac{-(g+m\,W+\alpha B/2)^2}{\alpha p\,r}}\rangle_W \qquad B = \frac{p}{(1-C)}\frac{1}{2}\,\mathrm{erfc}\Big(\frac{\theta}{\sqrt{2pq}}\Big) \end{split}$$

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Hopfield network with threshold

► The Hopfield model can be reproduced but with the presence of a threshold $(g=-\alpha B/2, L=1, p=1)$



The threshold (θ) can be increased to escape from the glassy phase of the Hopfield model.

The machine can learn again with an higher capacity α_c

Compositional phase

- ▶ Case of simulations: $L \sim \frac{l}{p}$ for p << 1. More than one hidden unit cooperate to generate data.
- ► Change of parameters:

$$\begin{cases} L = l/p \\ \theta = \tilde{\theta}\sqrt{p} \\ m = \tilde{m}\frac{p}{2} \\ q = \tilde{q}p \end{cases} \qquad \begin{cases} r = \tilde{r}p \\ B = \tilde{B}p \\ f = \tilde{f}p \end{cases}$$

$$\begin{cases} M = \frac{1}{2} \frac{\tilde{m}}{\sqrt{\alpha \tilde{r}}} \\ \theta_v = -\frac{\tilde{g} + \alpha \tilde{B}/2}{\sqrt{\alpha \tilde{r}}} \\ \theta_h = \tilde{\theta}/\sqrt{q} \end{cases}$$



Compositional phase

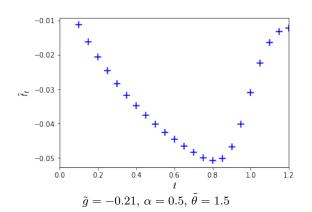
► Saddle point equations:

$$\begin{cases} \tilde{m} = \frac{2}{l} \langle W H^{(0)} \left(- (MW - \theta_v) \right) \rangle_W \\ C = \frac{1}{\sqrt{2\pi\alpha \tilde{r}}} \langle e^{-\frac{1}{2}(MW - \theta_v)^2} \rangle_W \\ q = \langle H^{(0)} \left(- (MW - \theta_v) \right) \rangle_W \\ \tilde{r} = \frac{q}{(1 - C)^2} H^{(2)}(\theta_h) \\ \tilde{B} = \frac{1}{(1 - C)} H^{(0)}(\theta_h) \end{cases}$$

Rescaled free energy

The new saddle point equations and the parameters give the rescaled free energy:

$$\tilde{f}_{GS} = -\frac{l}{8}\tilde{m}^2 - \frac{\alpha}{2}(\tilde{r}C + \tilde{B}q) - \tilde{g}q + \frac{\alpha\sqrt{q}}{2}\tilde{\theta}\frac{H^{(1)}\left(\frac{\tilde{\theta}}{\sqrt{q}}\right)}{1-C}$$



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Bibliography

- [1] J. Tubiana and R. Monasson, "Emergence of compositional representations in restricted boltzmann machines," *Physical review letters*, vol. 118, no. 13, p. 138 301, 2017.
- [2] D. J. Amit, H. Gutfreund, and H. Sompolinsky, "Storing infinite numbers of patterns in a spin-glass model of neural networks," *Physical Review Letters*, vol. 55, no. 14, p. 1530, 1985.
- [3] P. Mehta, M. Bukov, C.-H. Wang, A. G. Day, C. Richardson, C. K. Fisher, and D. J. Schwab, "A high-bias, low-variance introduction to machine learning for physicists," *Physics Reports*, vol. 810, pp. 1–124, May 2019, ISSN: 0370-1573. DOI: 10.1016/j.physrep.2019.03.001. [Online]. Available: http://dx.doi.org/10.1016/j.physrep.2019.03.001.
- [4] T. Castellani and A. Cavagna, "Spin-glass theory for pedestrians," Journal of Statistical Mechanics: Theory and Experiment, vol. 2005, no. 05, P05012, 2005.
- [5] D. J. Amit, H. Gutfreund, and H. Sompolinsky, "Spin-glass models of neural networks," *Physical Review A*, vol. 32, no. 2, p. 1007, 1985.

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Bibliography (cont.)

- [6] P. Dayan and L. F. Abbott, *Theoretical neuroscience:* computational and mathematical modeling of neural systems. Computational Neuroscience Series, 2001.
- [7] J. Son, "Replica trick on spin glasses and boolean satisfiability,", 2018.
- [8] J. Tubiana, "Restricted boltzmann machines: From compositional representations to protein sequence analysis," Ph.D. dissertation, PSL Research University, 2018.
- [9] D. J. MacKay and D. J. Mac Kay, *Information theory, inference and learning algorithms*. Cambridge university press, 2003.
- [10] M. Mezard and A. Montanari, *Information, physics, and computation*. Oxford University Press, 2009.
- [11] J. Schlüter, "Restricted boltzmann machine derivations," Technical Report TR-2014-13, Österreichisches Forschungsinstitut für ..., Tech. Rep., 2014.

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