The Helmholtz Machine

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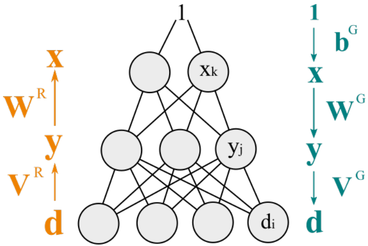

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Summary

INTRODUCTION

- The Helmholtz machine (HM) is a **probabilistic model** that is trained to create a generative model of a dataset
- It attempts to build a probability density models of the input data
- Main characteristics:
  - The network is composed by "two binary nets"
  - The training phase also has two parts (wake and sleep phases)
  - The whole learning is carried out by an unsupervised method
  - It is based on the statistical physics and information theory
  - Heavily related with the restricted Boltzmann machine

PROBABILITY

- Let us consider a bit vector $\mathbf{d} \in \{0, 1\}^N$
  - Where N is the nº of bits
  - Ex: $N = 2 \rightarrow \mathbf{d} = \{00, 01, 10, 11\}$
- The HM is all about assigning probabilities to bit vectors like $\mathbf{d}$
  - $p : \{0, 1\}^N \rightarrow [0, 1]$ with $p(\mathbf{d}) \geq 0$ and $\sum_{\mathbf{d}} = 1$
  - $p(\mathbf{d}_1), p(\mathbf{d}_2), \ldots, p(\mathbf{d}_N)$
- Such probability assignment gives the distribution of a discrete random variable $\mathbf{D}$
  - $p(\mathbf{d}) = \text{Prob}\,[\mathbf{D} = \mathbf{d}]$
  - *The probability that the random bit vector* $\mathbf{D}$ *takes on specific value* $\mathbf{d}$

PROBABILITY

- Considering a pair of bit vectors:
  - $p : \{0,1\}^L \times \{0,1\}^M \rightarrow [0,1]$
  - We describe it as $p(\mathbf{x}, \mathbf{y})$
- The joint probability distribution of two random bit vectors $\mathbf{X}$ and $\mathbf{Y}$
  - $p(\mathbf{x}, \mathbf{y}) = \text{Prob}[\mathbf{X} = \mathbf{x} \text{ and } \mathbf{Y} = \mathbf{y}]$
- Several definitions come from this distribution:
  - Marginalization
    - $p(\mathbf{x}) = \sum_{\mathbf{y}} p(\mathbf{x}, \mathbf{y})$ and $p(\mathbf{y}) = \sum_{\mathbf{x}} p(\mathbf{x}, \mathbf{y})$
  - Independence
    - $p(\mathbf{x}, \mathbf{y}) = p(\mathbf{x}).p(\mathbf{y})$
  - Conditional probability
    - $p(\mathbf{x}|\mathbf{y}) = \frac{p(\mathbf{x},\mathbf{y})}{p(\mathbf{y})}$

PROBABILITY

- From the previous definitions:
  - $p(\mathbf{x}, \mathbf{y}) = p(\mathbf{x}|\mathbf{y}).p(\mathbf{y})$
  - $p(\mathbf{x}) = \sum_{\mathbf{y}} p(\mathbf{x}|\mathbf{y}).p(\mathbf{y})$
  - $p(\mathbf{x}, \mathbf{y}|\mathbf{d}) = \frac{p(\mathbf{x},\mathbf{y},\mathbf{d})}{p(\mathbf{d})}$
  - $p(\mathbf{y}|\mathbf{x}) = \frac{p(\mathbf{y})}{p(\mathbf{x})}p(\mathbf{x}|\mathbf{y})$ (Bayes Theorem)

INDEPENDENT AND IDENTICALLY DISTRIBUTED RANDOM VARIABLES

- A random bit vector **D** with distribution p(**d**) can be described as a joint distribution over all N bits:
  - $\mathbf{d} : p(\mathbf{d}) = p(d_1, d_2, \ldots, d_N)$
- It is often the case in which that bit is independent and identically distributed (IID) random variable
  - They are mutually independent
    - $p(d_1, d_2, \ldots, d_N) = p(d_1)p(d_2)\ldots p(d_N)$
  - They are identically distributed
    - $p(d_i = 1) = p_0$ and $p(d_i = 0) = 1 - p_0$
- For any specific bit vector **d**:

$$p(\mathbf{d}) = \prod_i p_0^{d_i}(1 - p_0)^{1-d_i} \tag{1}$$

SURPRISE AND ENTROPY

- It is often convenient to recast a probability value p into a quantity called **surprise**

$$s = -\log(\mathbf{d}) \tag{2}$$

  - An event with $p = 1 \Rightarrow$ zero surprise
  - An event with $p = 0 \Rightarrow$ infinity surprise
  - Surprise is never negative

- Let us consider a function $f(\mathbf{D})$, where $\mathbf{D}$ is a random variable
  - The expectation value of this function is given by

$$\langle f(\mathbf{D}) \rangle = \sum_{\mathbf{d}} p(\mathbf{d}) f(\mathbf{d}) \tag{3}$$

SURPRISE AND ENTROPY

- The expected value of the surprise is called **entropy**

$$H(\mathbf{D}) = \langle -\log p(\mathbf{D}) \rangle = -\sum_{\mathbf{d}} p(\mathbf{d}) \log p(\mathbf{d}) \tag{4}$$

  where $\log 0 = 0$

- **Low** entropy $\Rightarrow$ **low** surprise $\Rightarrow$ the system's probabilities tend to be **uniform**

- **High** entropy $\Rightarrow$ **high** surprise $\Rightarrow$ the system's probabilities are **unequal**

- For conditional probabilities we have conditional entropy

$$H(\mathbf{X}|\mathbf{Y}) = -\sum_{\mathbf{d}} p(\mathbf{x}|\mathbf{y}) \log p(\mathbf{x}|\mathbf{y}) \tag{5}$$

KULLBACK-LEIBLER DIVERGENCE

- It is one way to quantify how different two probability distribution are

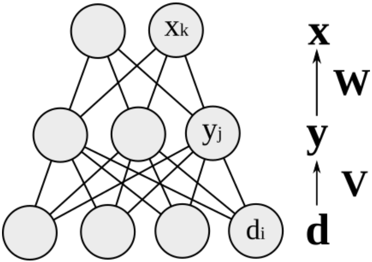
$$KL[p_A(\mathbf{D}), p_B(\mathbf{D})] = \sum_{\mathbf{d}} p_A(\mathbf{d}) \log \frac{p_A(\mathbf{d})}{p_B(\mathbf{d})} \tag{6}$$

- If $p_A(\mathbf{d}) = p_B(\mathbf{d}) \Rightarrow KL = 0$
- KL is never negative and $KL[p_A(\mathbf{D}), p_B(\mathbf{D})] \neq KL[p_B(\mathbf{D}), p_A(\mathbf{D})]$
- Using the logarithm's properties and the expectation value's definition

$$KL[p_A(\mathbf{D}), p_B(\mathbf{D})] = \langle -\log p_B(\mathbf{D}) \rangle_A - \langle -\log p_A(\mathbf{D}) \rangle_A \tag{7}$$

- Thus, the KL from A to B is simply the difference in surprise averaged by A.

LAYERED NEURAL NETWORKS



- Each neuron computes:

$$d_i = \sum_{j=1}^{L} w_{ij} y_j + b_j^d \tag{8}$$

$$y_j = \sum_{k=1}^{L} w_{jk} x_k + b_k^y \tag{9}$$

- To ease the computation we attach the bias into **W** and **V** and appened 1 at the end of **x** and **y**
- Adding a nonlinearity: $\mathbf{y} = \sigma(\mathbf{W}\mathbf{x})$ and $\mathbf{y} = \sigma(\mathbf{V}\mathbf{y})$
  - Where $\sigma(a) = \frac{1}{1+e^{-a}}$

LAYERED NEURAL NETWORKS

- Due to the sigmoid, the neuron output value is in [0,1]
- We can interpret this value as the probability that a binary-value neuron produces the output 1
  - The probability it *"fires"* or *"turn on"*

$$\mathbf{y} = \text{sample}\left[p_y\right], \text{where } p_y = \sigma(\mathbf{W}\mathbf{x}) \tag{10}$$

$$\mathbf{d} = \text{sample}\left[p_d\right], \text{where } p_d = \sigma(\mathbf{V}\mathbf{y}) \tag{11}$$

- Sample $[p]$ is a stochastic function that yields 1 with probability p and 0 with $1 - p$
- As σ never reaches 0 or 1, a neuron will never *fire* with complete certainty
- This layered stochastic network will be the starting point for the Helmholtz machine

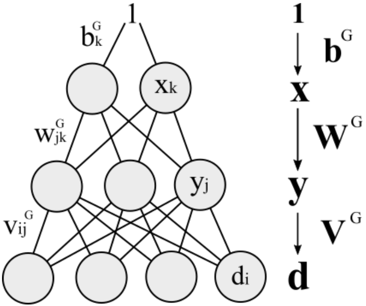
TOP-DOWN PATTERN GENERATION

- The HM sees the world as patterns made of flickering bits
  - Each bit pattern $\mathbf{d}$ appears with $p(\mathbf{d})$
- Since $\mathbf{d}$ can assume a huge number os values, specifying $p\mathbf{d}$ requires a lot of information
  - However, the world is not completly random and the HM attempts to exploit it
- In order to determine the data distribution $p(\mathbf{d})$ we do the following:
  1. From a generative distribution we produce $\mathbf{d}$ using the chain $\mathbf{1} \to \mathbf{x} \to \mathbf{y} \to \mathbf{d}$
  2. This chain will be implemented as a layered neural network

TOP-DOWN PATTERN GENERATION

3. The pattern **x** is stochastically generated from a constant bias
   - It is not regarded to the input network

4. Only the layer **d** is connected to the real data. **x** and **y** are hidden layers



TOP-DOWN PATTERN GENERATION

- A generative distribution G for our chain requires the sprecification of three distributions:
  - $p_G(\mathbf{x})$, $p_G(\mathbf{y}|\mathbf{x})$ and $p_G(\mathbf{d}|\mathbf{y})$
- Writing the chain $\mathbf{x} \rightarrow \mathbf{y} \rightarrow \mathbf{d}$ is a way to say we have conditional independence of $\mathbf{x}$ and $\mathbf{d}$ given $\mathbf{y}$:

$$p_G(\mathbf{x}, \mathbf{d}|\mathbf{y}) = p_G(\mathbf{x}|\mathbf{y}) p_G(\mathbf{d}|\mathbf{y}) \tag{12}$$

- In other words, $\mathbf{x}$ inlfuences $\mathbf{d}$ only through $\mathbf{y}$:

$$p_G = (\mathbf{d}|\mathbf{x}, \mathbf{y}) = p_G(\mathbf{d}|\mathbf{y}) \tag{13}$$

TOP-DOWN PATTERN GENERATION

- From Eq. 12:

$$
\begin{gathered}
p_G(\mathbf{d}|\mathbf{y}) = \frac{p_G(\mathbf{x},\mathbf{d}|\mathbf{y})}{p_G(\mathbf{x}|\mathbf{y})} \\
p_G(\mathbf{x},\mathbf{y},\mathbf{d}) = p_G(\mathbf{y},\mathbf{d}|\mathbf{x})p_G(\mathbf{x})
\end{gathered} \tag{14}
$$

- From Eq. 14 we can get the 3 generation distributions required:

$$
\begin{gathered}
p_G(\mathbf{x},\mathbf{y},\mathbf{d}) = p_G(\mathbf{y},\mathbf{d}|\mathbf{x})p_G(\mathbf{x}) \\
p_G(\mathbf{x},\mathbf{y},\mathbf{d}) = [p_G(\mathbf{d}|\mathbf{x},\mathbf{y})p_G(\mathbf{y}|\mathbf{x})]p_G(\mathbf{x}) \\
\boxed{p_G(\mathbf{x},\mathbf{y},\mathbf{d}) = p_G(\mathbf{d}|\mathbf{y})p_G(\mathbf{y}|\mathbf{x})p_G(\mathbf{x})}
\end{gathered} \tag{15}
$$

TOP-DOWN PATTERN GENERATION

- Moreover, we can get them only from the joint distribution:

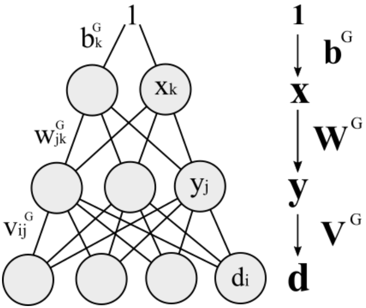
$$p_G(\mathbf{x}) = \sum_{\mathbf{y},\mathbf{d}} p_G(\mathbf{x}, \mathbf{y}, \mathbf{d})$$

$$p_G(\mathbf{y}|\mathbf{x}) = \frac{p_G(\mathbf{x},\mathbf{y})}{p_G(\mathbf{x})} = \frac{\sum_{\mathbf{d}} p_G(\mathbf{x},\mathbf{y},\mathbf{d})}{\sum_{\mathbf{y},\mathbf{d}} p_G(\mathbf{x},\mathbf{y},\mathbf{d})} \tag{16}$$

$$p_G(\mathbf{d}|\mathbf{y}) = \frac{p_G(\mathbf{d},\mathbf{y})}{p_G(\mathbf{y})} = \frac{\sum_{\mathbf{d}} p_G(\mathbf{x},\mathbf{y},\mathbf{d})}{\sum_{\mathbf{x},\mathbf{d}} p_G(\mathbf{x},\mathbf{y},\mathbf{d})}$$

- Thus, we just speak of $p_G(\mathbf{x}, \mathbf{y}, \mathbf{d})$ as the generative distribution pack
- The ultimate quatity of interest is $p_G(\mathbf{d})$
  - The goal is to make the network's $p_G(\mathbf{d})$ as close as possible to the real data distribution $p(\mathbf{d})$

THE GENERATIVE MODEL AS A NEURAL NETWORK



- The set of connections $\{\mathbf{b}^G, \mathbf{W}^G, \mathbf{V}^G\}$ is a **way to specify** $p_G(\mathbf{x}, \mathbf{y}, \mathbf{d})$
  - Of course, it is a **constrained** form for a probability distribution
  - The machine attempts to **approximate** it as much as possible to the reality
- We get the directional probabilities using Eq. 1 and the weights:

$$p_G(\mathbf{x}) = \prod_k p_G(x_k)^{x_k}[1 - p_G(x_k)]^{1-x_k}, \text{ where } p_G(x_k) = \sigma(b_k^G) \tag{17}$$

THE GENERATIVE MODEL AS A NEURAL NETWORK

$$p_G(\mathbf{y}|\mathbf{x}) = \prod_k p_G(y_j|x)^{y_j}[1-p_G(y_j|x)]^{1-y_j}, \text{ where: } p_G(y_j|x) = \sigma(\sum_{k=1}^{L} w^G_{jk}x_k) \tag{18}$$

$$p_G(\mathbf{d}|\mathbf{y}) = \prod_k p_G(d_i|y)^{d_i}[1-p_G(d_i|y)]^{1-d_i}, \text{ where: } p_G(d_i|y) = \sigma(\sum_{j=1}^{M} v^G_{ij}y_j) \tag{19}$$

- **x** and **y** are known as the explanation of **d**
- The number of neurons are unrestricted
- There are variants with more layers, different activation functions, lateral connections and so on

ENERGY

- Let us consider the probability of an explanation $\mathbf{x}$ and $\mathbf{y}$ given some fixed piece of generated data $\mathbf{d}$:

$$p_G(\mathbf{x}, \mathbf{y}|\mathbf{d}) = \frac{p_G(\mathbf{x}, \mathbf{y}, \mathbf{d})}{p_G(\mathbf{d})} = \boxed{\frac{p_G(\mathbf{x}, \mathbf{y}, \mathbf{d})}{\sum_{\mathbf{xy}} p_G(\mathbf{x}, \mathbf{y}, \mathbf{d})}} \tag{20}$$

- According to the statistical physics, this is a energy function:

$$E_G(\mathbf{x}, \mathbf{y}|\mathbf{d}) = -\log p_G(\mathbf{x}, \mathbf{y}, \mathbf{d}) \text{ Applying Eq. 20:}$$

$$p_G(\mathbf{x}, \mathbf{y}|\mathbf{d}) = \frac{e^{-E_G(\mathbf{x}, \mathbf{y}|\mathbf{d})}}{\sum_{\mathbf{xy}} e^{-E_G(\mathbf{x}, \mathbf{y}|\mathbf{d})}} \tag{21}$$

ENERGY

- From the generative energy $E_G(\mathbf{x}, \mathbf{y}|\mathbf{d})$ an analogy to statistical physics arises:
  - Suppose the state of a physical system fluctuates among a set of state $\{q_1, q_2, \ldots\}$
  - The system is in **thermal equilibrium** if the probability of finding the system in a state q_i is related to its energy $E(q_i)$
  - This energy behaves according to the **Boltzmann distribution**

$$p(q_i) = \frac{e^{-\frac{E(q_i)}{T}}}{\sum_i e^{-\frac{E(q_i)}{T}}} \tag{22}$$

- Taking $T = 1$, $E_G(\mathbf{x}, \mathbf{y}|\mathbf{d})$ is known as the energy of the explanation **x, y** of the data pattern **d**
- The energy is the **surprise associated** with the ocurrence of a **particular complete state**

FREE ENERGY

- We want to find a generative model, i.e, $\{\mathbf{b}^G, \mathbf{W}^G, \mathbf{V}^G\}$, that makes $p_G(\mathbf{d})$ close to $p(\mathbf{d})$. Therefore:

$$\phi(G) = KL[p(\mathbf{D}), p_G(\mathbf{D})]$$

$$\phi(G) = \sum_{\mathbf{d}} p(\mathbf{d}) \log \frac{p(\mathbf{d})}{p_G(\mathbf{d})} = \sum_{\mathbf{d}} p(\mathbf{d}) \log p(\mathbf{d}) - \boxed{\sum_{\mathbf{d}} p(\mathbf{d}) \log p_G(\mathbf{d})} \tag{23}$$

- It is the expected surprise of the of the data generated by the network weighted by the real-world probability data:

$$\phi_2(G) = \sum_{\mathbf{d}} p(\mathbf{d}) \log p_G(\mathbf{d}) = \langle -\log p_G(\mathbf{D}) \rangle \tag{24}$$

- The surprise will get smaller if the HM learns a model that is close to $p(\mathbf{d})$

FREE ENERGY

- Thus, our optimization problem is to minimize $\phi_2(G)$:

$$\nabla\phi_2(G) = \sum_{\mathbf{d}} p(\mathbf{d}) \boxed{\nabla[\log p_G(\mathbf{d})]} \tag{25}$$

  - We need to focus on the boxed part of Eq. 25

$$\begin{aligned}
-\log p_G(\mathbf{d}) &= -\log p_G(\mathbf{d}) \times 1 \\
-\log p_G(\mathbf{d}) &= -\log p_G(\mathbf{d})[\textstyle\sum_{\mathbf{x},\mathbf{y}} p_G(\mathbf{x},\mathbf{y}|\mathbf{d})] \\
-\log p_G(\mathbf{d}) &= -\textstyle\sum_{\mathbf{x},\mathbf{y}} p_G(\mathbf{x},\mathbf{y}|\mathbf{d}) \log p_G(\mathbf{d}) \\
-\log p_G(\mathbf{d}) &= -\textstyle\sum_{\mathbf{x},\mathbf{y}} p_G(\mathbf{x},\mathbf{y}|\mathbf{d}) \log[\frac{p_G(\mathbf{x},\mathbf{y},\mathbf{d})}{p_G(\mathbf{x},\mathbf{y}|\mathbf{d})}] \\
-\log p_G(\mathbf{d}) &= -\textstyle\sum_{\mathbf{x},\mathbf{y}} p_G(\mathbf{x},\mathbf{y}|\mathbf{d}) \log p_G(\mathbf{x},\mathbf{y},\mathbf{d}) + -\sum_{\mathbf{x},\mathbf{y}} p_G(\mathbf{x},\mathbf{y}|\mathbf{d}) \log p_G(\mathbf{x},\mathbf{y}|\mathbf{d}) \\
-\log p_G(\mathbf{d}) &= -\textstyle\sum_{\mathbf{x},\mathbf{y}} p_G(\mathbf{x},\mathbf{y}|\mathbf{d}) E_G(\mathbf{x},\mathbf{y}|\mathbf{d}) + H_G(\mathbf{X},\mathbf{Y}|\mathbf{d}) \\
-\log p_G(\mathbf{d}) &= \boxed{\langle E_G(\mathbf{X},\mathbf{Y};\mathbf{d})\rangle_G - H_G(\mathbf{X},\mathbf{Y}|\mathbf{d})}
\end{aligned} \tag{26}$$

- In statistical physics, the **Helmholtz free energy** of a system is given by $F = \langle E \rangle - TH$

FREE ENERGY

- Thus, taking $T = 1$:

$$F_G(\mathbf{d}) = -\log p_G(\mathbf{d}) = \langle E_G(\mathbf{X}, \mathbf{Y}; \mathbf{d})\rangle_G - H_G(\mathbf{X}, \mathbf{Y}|\mathbf{d}) \tag{27}$$

- So, minimizing the KL divergence means minimizing the generative free energy $F_G(\mathbf{D})$:

$$\frac{\partial}{\partial b_k^G} F_G(\mathbf{d}) \quad \frac{\partial}{\partial w_{jk}^G} F_G(\mathbf{d}) \quad \frac{\partial}{\partial v_{jk}^G} F_G(\mathbf{d}) \tag{28}$$

- We need to express $F_G(\mathbf{D})$ in terms of the weights, however:
  - It does not work very well
  - The equations are very hard to manipulate

VARIATIONAL FREE ENERGY

- Let us consider another distribution $p_R(\mathbf{x}, \mathbf{y}|\mathbf{d})$, which can be any arbitrary distribution for the moment

- Let us compute:

$$
\begin{gathered}
KL[p_R(\mathbf{X}, \mathbf{Y}|\mathbf{d}), p_G(\mathbf{X}, \mathbf{Y}|\mathbf{d})] = \sum_{\mathbf{xy}} p_R(\mathbf{xy}|\mathbf{d}) \log \frac{p_R(\mathbf{x},\mathbf{y}|\mathbf{d})}{p_G(\mathbf{x},\mathbf{y}|\mathbf{d})} \\
KL[p_R(\mathbf{X}, \mathbf{Y}|\mathbf{d}), p_G(\mathbf{X}, \mathbf{Y}|\mathbf{d})] = -H_R(\mathbf{X}, \mathbf{Y}|\mathbf{d}) + \langle E_G(\mathbf{X}, \mathbf{Y}; \mathbf{d}) \rangle_R - F_G(\mathbf{d}) \\
\boxed{F_G(\mathbf{d}) = -H_R(\mathbf{X}, \mathbf{Y}|\mathbf{d}) + \langle E_G(\mathbf{X}, \mathbf{Y}; \mathbf{d}) \rangle_R - KL[p_R(\mathbf{X}, \mathbf{Y}|\mathbf{d}), p_G(\mathbf{X}, \mathbf{Y}|\mathbf{d})]}
\end{gathered}
\tag{29}
$$

- Now he have a expression for the generative Helmholtz free energy involving a new distribution p_R

- To proceed we need to use a method called *variational method*

VARIATIONAL FREE ENERGY

- Since the KL cannot be negative:

$$\begin{gathered} -H_R(\mathbf{X}, \mathbf{Y}|\mathbf{d}) + \langle E_G(\mathbf{X}, \mathbf{Y}; \mathbf{d})\rangle_R - F_G(\mathbf{d}) \geq 0 \\ F_G(\mathbf{d}) \leq \langle E_G(\mathbf{X}, \mathbf{Y}; \mathbf{d})\rangle_R - H_R(\mathbf{X}, \mathbf{Y}|\mathbf{d}) \end{gathered} \tag{30}$$

- The variational free energy from R to G is defined as:

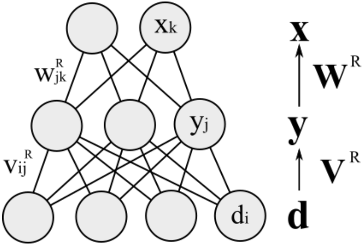
$$\begin{gathered} F_G^R(\mathbf{d}) = \langle E_G(\mathbf{X}, \mathbf{Y}; \mathbf{d})\rangle_R - H_R(\mathbf{X}, \mathbf{Y}|\mathbf{d}) \\ F_G^R(\mathbf{d}) = F_G(\mathbf{d}) + KL[p_R(\mathbf{X}, \mathbf{Y}|\mathbf{d}), p_G(\mathbf{X}, \mathbf{Y}|\mathbf{d})] \end{gathered} \tag{31}$$

  - Note that $F_G^G(\mathbf{d}) = F_G(\mathbf{d})$

- Now we need to provide a method to determine $p_R(\mathbf{X}, \mathbf{Y}|\mathbf{d})$

BOTTOM-UP PATTERN RECOGNITION

- In order to determine $p_R(\mathbf{x}, \mathbf{y}|\mathbf{d})$, let us assume the chain $\mathbf{d} \rightarrow \mathbf{x} \rightarrow \mathbf{y}$
  - It means we can factor $p_R(\mathbf{x}, \mathbf{y}|\mathbf{d}) = p_R(\mathbf{x}|\mathbf{y})p_R(\mathbf{y}|\mathbf{d})$
- As previously, let us use the HM upward connections to help us with this task



BOTTOM-UP PATTERN RECOGNITION

- The pattern **d** is the network input, and there is no bias weight coming into it
- Thus, unlike the generative case, we have only two equations:

$$p_R(\mathbf{x}|\mathbf{y}) = \prod_k p_R(x_k|y)^{x_k}[1 - p_R(x_k|y)]^{1-x_k}, \text{ where: } p_R(x_k|y) = \sigma(\sum_{j=1}^{M} w_{kj}^R y_j) \tag{32}$$

$$p_R(\mathbf{y}|\mathbf{d}) = \prod_j p_R(y_j|d)^{y_j}[1 - p_R(y_j|d)]^{1-y_j}, \text{ where: } p_R(y_j|d) = \sigma(\sum_{i=1}^{N} v_{ji}^R d_i) \tag{33}$$

LEARNING

- The HM learning algorithm is based on gradient descent and it will involve two phases:
  1. **Wake-phase:** it involves the generative weights

$$F_G^R(\mathbf{d}) = F_G(\mathbf{d}) + KL[p_R(\mathbf{X}, \mathbf{Y}|\mathbf{d}), p_G(\mathbf{X}, \mathbf{Y}|\mathbf{d})] \tag{34}$$

  2. **Sleep-phase:** it involves the recognition weights

$$\tilde{F}_G^R(\mathbf{d}) = F_G(\mathbf{d}) + KL[p_G(\mathbf{X}, \mathbf{Y}|\mathbf{d}), p_R(\mathbf{X}, \mathbf{Y}|\mathbf{d})] \tag{35}$$

- Both phase use the variational free energy to compute the gradients

LEARNING: WAKE-PHASE

- In this pahse we need to work with $F_G^R(\mathbf{d})$:

$$\begin{aligned} F_G^R(\mathbf{d}) &= \langle E_G(\mathbf{X},\mathbf{Y};\mathbf{d})\rangle_R - H_R(\mathbf{X},\mathbf{Y}|\mathbf{d}) \\ F_G^R(\mathbf{d}) &= \boxed{\sum_{\mathbf{xy}} p_R(\mathbf{x},\mathbf{y}|\mathbf{d})E_G(\mathbf{x},\mathbf{y};\mathbf{d})} - H_R(\mathbf{X},\mathbf{Y}|\mathbf{d}) \end{aligned} \tag{36}$$

- Let us take the derivatives $\frac{\partial}{\partial b^G}$, $\frac{\partial}{\partial w^G_{jk}}$ and $\frac{\partial}{\partial v^G_{ij}}$ as ∇_G:

$$\begin{aligned} \nabla_G F_G^R(\mathbf{d}) &= \nabla_G \textstyle\sum_{\mathbf{xy}} p_R(\mathbf{x},\mathbf{y}|\mathbf{d})E_G(\mathbf{x},\mathbf{y};\mathbf{d}) \\ \nabla_G F_G^R(\mathbf{d}) &= \textstyle\sum_{\mathbf{xy}} p_R(\mathbf{x},\mathbf{y}|\mathbf{d})\nabla_G E_G(\mathbf{x},\mathbf{y};\mathbf{d}) \\ \nabla_G F_G^R(\mathbf{d}) &= \langle \nabla_G E_G(\mathbf{X},\mathbf{Y};\mathbf{d})\rangle_R \end{aligned} \tag{37}$$

- Thus, the algorithm will sample a pattern **d** from the recognition phase then updates the weights throught a small gradient step

LEARNING: WAKE-PHASE

- Now we need to evaluate $\nabla_G E_G$:

$$
\begin{aligned}
\nabla_G \nabla_G E_G(\mathbf{X}, \mathbf{Y}; \mathbf{d}) &= -\nabla_G \log p_G(\mathbf{x}, \mathbf{y}, \mathbf{d}) \\
\nabla_G \nabla_G E_G(\mathbf{X}, \mathbf{Y}; \mathbf{d}) &= -\nabla_G \log p_G(\mathbf{x}) p_G(\mathbf{y}|\mathbf{x}) p_G(\mathbf{d}|\mathbf{y}) \\
\nabla_G \nabla_G E_G(\mathbf{X}, \mathbf{Y}; \mathbf{d}) &= \boxed{-\nabla_G \log p_G(\mathbf{x}) - \nabla_G \log p_G(\mathbf{y}|\mathbf{x}) - \nabla_G \log p_G(\mathbf{d}|\mathbf{y})}
\end{aligned}
\tag{38}
$$

- According to our model:

$$
\begin{aligned}
\log p_G(\mathbf{x}) &= \log \textstyle\prod_k \xi_k^{x_k} (1-\xi_k)^{1-x_k}, \text{ where } \xi_k = \sigma(b_k^G) \\
\log p_G(\mathbf{x}) &= \textstyle\sum_k x_k \log \xi_k + \sum_k (1-x_k) \log(1-\xi_k) \\
\log p_G(\mathbf{y}|\mathbf{x}) &= \log \textstyle\prod_j \psi_j^{y_j} (1-\psi_j)^{1-y_j}, \text{ where } \psi_j = \sigma(\sum_{k=1}^{L} w_{jk}^G x_k) \\
\log p_G(\mathbf{y}|\mathbf{x}) &= \textstyle\sum_j y_j \log \psi_j + \sum_j (1-y_j) \log(1-\psi_j) \\
\log p_G(\mathbf{d}|\mathbf{y}) &= \log \textstyle\prod_i \delta_i^{d_i} (1-\delta_i)^{1-d_i}, \text{ where } \delta_i = \sigma(\sum_{j=1}^{M} v_{jk}^G y_j) \\
\log p_G(\mathbf{d}|\mathbf{y}) &= \textstyle\sum_i d_i \log \delta_i + \sum_i (1-d_i) \log(1-\delta_i)
\end{aligned}
\tag{39}
$$

LEARNING: WAKE-PHASE

- Computing the derivatives (hint: $a = \sigma(b) \Rightarrow \frac{\mathrm{d}a}{\mathrm{d}b} = a(1-a)$)

$$
\begin{aligned}
\frac{\partial \log p_G(\mathbf{x})}{\partial b_k^G} &= \frac{\partial}{\partial b_k^G} \sum_k x_k \log \xi_k + \frac{\partial}{\partial b_k^G} \sum_k (1-x_k) \log(1-\xi_k) \\
\frac{\partial \log p_G(\mathbf{x})}{\partial b_k^G} &= \frac{\partial}{\partial b_k^G} [x_k \log \xi_k] + \frac{\partial}{\partial b_k^G} [(1-x_k) \log(1-\xi_k)] \\
\frac{\partial \log p_G(\mathbf{x})}{\partial b_k^G} &= x_k \frac{\partial}{\partial b_k^G} \log \xi_k + (1-x_k) \frac{\partial}{\partial b_k^G} \log(1-\xi_k) \\
\frac{\partial \log p_G(\mathbf{x})}{\partial b_k^G} &= \frac{x_k}{\xi_k} \frac{\partial}{\partial b_k^G} \xi_k + \frac{(1-x_k)}{(1-\xi_k)} \frac{\partial}{\partial b_k^G} (1-\xi_k) \\
\frac{\partial \log p_G(\mathbf{x})}{\partial b_k^G} &= \frac{x_k}{\xi_k} \frac{\partial}{\partial b_k^G} \xi_k - \frac{(1-x_k)}{(1-\xi_k)} \frac{\partial}{\partial b_k^G} \xi_k \\
\frac{\partial \log p_G(\mathbf{x})}{\partial b_k^G} &= \frac{x_k}{\xi_k} \frac{\partial}{\partial b_k^G} \xi_k - \frac{(1-x_k)}{(1-\xi_k)} \frac{\partial}{\partial b_k^G} \xi_k \text{ **hint} \\
\frac{\partial \log p_G(\mathbf{x})}{\partial b_k^G} &= \frac{x_k}{\xi_k} \xi_k (1-\xi_k) - \frac{(1-x_k)}{(1-\xi_k)} \xi_k (1-\xi_k) \\
\frac{\partial \log p_G(\mathbf{x})}{\partial b_k^G} &= \boxed{x_k - \xi_k}
\end{aligned}
\tag{40}
$$

LEARNING: WAKE-PHASE

$$\frac{\partial \log p_G(\mathbf{y}|\mathbf{x})}{\partial b_k^G} = 0 \quad \frac{\partial \log p_G(\mathbf{d}|\mathbf{y})}{\partial b_k^G} = 0 \tag{41}$$

- The remaining derivatives are computed similarity to Eq. 40

$$\frac{\partial \log p_G(\mathbf{y}|\mathbf{x})}{\partial w_{jk}^G} = (y_j - \psi_j)x_k \quad \frac{\partial \log p_G(\mathbf{d}|\mathbf{y})}{\partial w_{jk}^G} = 0 \quad \frac{\partial \log p_G(\mathbf{x})}{\partial w_{jk}^G} = 0 \tag{42}$$

$$\frac{\partial \log p_G(\mathbf{d}|\mathbf{y})}{\partial v_{ij}^G} = (d_i - \delta_i)y_j \quad \frac{\partial \log p_G(\mathbf{d}|\mathbf{y})}{\partial v_{ij}^G} = 0 \quad \frac{\partial \log p_G(\mathbf{x})}{\partial v_{ij}^G} = 0 \tag{43}$$

- In a vectorial form:

$$\begin{aligned} \nabla_{\mathbf{b}^G} E_G(\mathbf{x},\mathbf{y};\mathbf{d}) &= -(\mathbf{x} - \xi) \\ \nabla_{\mathbf{W}^G} E_G(\mathbf{x},\mathbf{y};\mathbf{d}) &= -(\mathbf{y} - \psi)\mathbf{x}^T \\ \nabla_{\mathbf{V}^G} E_G(\mathbf{x},\mathbf{y};\mathbf{d}) &= -(\mathbf{d} - \delta)\mathbf{y}^T \end{aligned} \tag{44}$$

LEARNING: WAKE-PHASE

- **b** comes to the world
- **x** and **y** come from the recognition distribution given **d**
- ξ, ψ and δ come from the generative distribution given **x** and **y**
- For each layer, the update rules are:

$$\begin{aligned} \mathbf{b}^G &+= \alpha(\mathbf{x} - \xi) \\ \mathbf{W}^G &+= \alpha(\mathbf{y} - \psi)\mathbf{x}^T \\ \mathbf{V}^G &+= \alpha(\mathbf{d} - \delta)\mathbf{y}^T \end{aligned} \tag{45}$$

where α is the learning rate

LEARNING: WAKE-PHASE

- Pseudocode for wake-phase:

Algorithm 1: Wake-phase

$\mathbf{d}$ = getSampleFromWorld()

$\mathbf{y} = \text{sample}\,[\sigma(\mathbf{V}^R\mathbf{d}^T)]$

$\mathbf{x} = \text{sample}\,[\sigma(\mathbf{W}^R\mathbf{y}^T)]$

$\xi = \sigma(\mathbf{b}^G)$

$\psi = \sigma(\mathbf{W}^G\mathbf{x}^T)$

$\delta = \sigma(\mathbf{V}^G\mathbf{y}^T)$

$\mathbf{b}^G + = \alpha(\mathbf{x} - \xi)$

$\mathbf{W}^G + = \alpha(\mathbf{y} - \psi)\mathbf{x}^T$

$\mathbf{V}^G + = \alpha(\mathbf{d} - \psi)\mathbf{y}^T$

LEARNING: SLEEP-PHASE

- It is similar to wake-phase, but the derivatives are taken from $\tilde{F}_G^R(\mathbf{d}) = F_G(\mathbf{d}) + KL[p_G(\mathbf{X},\mathbf{Y}|\mathbf{d}), p_R(\mathbf{X},\mathbf{Y}|\mathbf{d})]$

$$\begin{aligned} \nabla_R \tilde{F}_G^R(\mathbf{d}) &= \quad KL[p_G(\mathbf{X},\mathbf{Y}|\mathbf{d}), p_R(\mathbf{X},\mathbf{Y}|\mathbf{d})] \\ \nabla_R \tilde{F}_G^R(\mathbf{d}) &= \qquad \langle \nabla_R \log p_R(\mathbf{X},\mathbf{Y}|\mathbf{d}) \rangle_G \end{aligned} \tag{46}$$

- Thus, we need to drawn our attention to $\nabla_R \log p_R(\mathbf{X},\mathbf{Y}|\mathbf{d})$
- The equations for $p_R(\mathbf{x}|\mathbf{y})$ and $p_R(\mathbf{y}|\mathbf{d})$ are obtained just like Eq. 39

LEARNING: SLEEP-PHASE

- The derivatives for $\log p_R(\mathbf{x}|\mathbf{y})$ and $\log p_R(\mathbf{y}|\mathbf{d})$ are obtained similarly to the wake-phase

$$\frac{\partial \log p_R(\mathbf{x}|\mathbf{y})}{\partial w^R_{kj}} = (x_k - \xi_k)x_j \qquad \frac{\partial \log p_R(\mathbf{y}|\mathbf{d})}{\partial w^R_{kj}} = 0 \tag{47}$$

$$\frac{\partial \log p_R(\mathbf{x}|\mathbf{y})}{\partial v^R_{ij}} = 0 \qquad \frac{\partial \log p_R(\mathbf{y}|\mathbf{d})}{\partial v^R_{ij}} = (y_j - \psi_k)d_i \tag{48}$$

- In a vectorial form:

$$\begin{aligned} \nabla_{\mathbf{W}^R} \log p_R(\mathbf{x}|\mathbf{y}) &= (\mathbf{x} - \xi)\mathbf{y}^T \\ \nabla_{\mathbf{V}^R} \log p_R(\mathbf{y}|\mathbf{d}) &= (\mathbf{y} - \psi)\mathbf{d}^T \end{aligned} \tag{49}$$

LEARNING: SLEEP-PHASE

- For each layer, the update rules are:

$$\begin{aligned} \mathbf{W}^R &+= \alpha(\mathbf{x} - \xi)\mathbf{y}^T \\ \mathbf{R}^G &+= \alpha(\mathbf{y} - \psi)\mathbf{d}^T \end{aligned} \tag{50}$$

where α is the learning rate

  - $\mathbf{x}$ and $\mathbf{y}$ come from the generative distribution
  - ξ and ψ come from the recognition distribution given $\mathbf{x}$ and $\mathbf{y}$

LEARNING: SLEEP-PHASE

- Pseudocode for sleep-phase:

Algorithm 2: Wake-phase

$\mathbf{x} = \text{sample}[\sigma(\mathbf{b}^G)]$

$\mathbf{y} = \text{sample}\ [\sigma(\mathbf{W}^G \mathbf{x}^T)]$

$\mathbf{d} = \text{sample}\ [\sigma(\mathbf{V}^G \mathbf{y}^T)]$

$\psi = \sigma(\mathbf{V}^R \mathbf{d}^T)$

$\xi = \sigma(\mathbf{W}^R \mathbf{y}^T)$

$\mathbf{V}^R + = \alpha(\mathbf{y} - \psi)\mathbf{d}^T$

$\mathbf{W}^R + = \alpha(\mathbf{x} - \xi)\mathbf{y}^T$

LEARNING: THE WHOLE ALGORITHM

- All weights are started at 0
  - As $\sigma(0) = 0.5$, every neuron has 50-50% change to fire

Algorithm 3: The whole algorithm

$\mathbf{W}^G, \mathbf{V}^G, \mathbf{b}^G = 0$

$\mathbf{W}^R, \mathbf{V}^R$

repeat

  wake-phase to change $\mathbf{W}^G, \mathbf{V}^G, \mathbf{b}^G$

  sleep-phase to change $\mathbf{V}^R, \mathbf{W}^R$

until *Stopping criteria*;

INSIGTHS

- The restricted Boltzmann machine shares some core concepts:
  - It is a generative model
  - Two training phases (positive and negative)
  - Based on energy functions

- Boltzmann machines use symmetrical weights for recognition and reconstruction whereas in Helmholtz machines the weights organization is different

INSIGTHS

- There is a theory that dreams are samples from a generative model that we generate in order to train the model to be better
- It happens with the RBM, HM and GANs
- So, GANs are also related to the wake-sleep procedure

NEXT STEPS

- Is the RBM a better model than HM?
  - What is the relationship between algorithm wake-sleep and contrastive divergence? Which one is better?
- Is it possible to use some concepts from the wake-sleep to improve the CNN training phase?
  - CNN-RBM-ELM
- Is the capsule network related to RBM and HM training phase?

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