

Boltzmann Machine

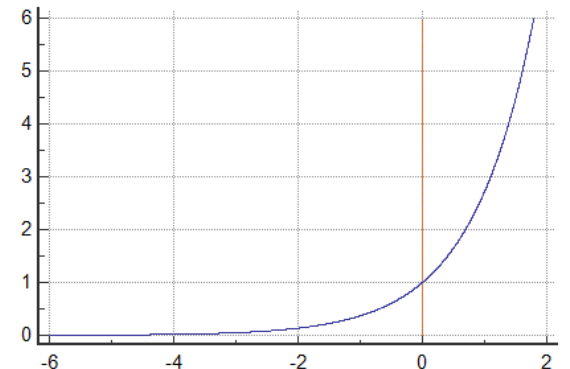
CS385 Machine Learning – Artificial Neural Network

Remembering process with SA (Rev.)

- HNN, 3 nodes, the status of each neuron is either 0 or 1
- consider neuron 1, its status S_1 is 1, to determine if it changed to $S_1'(0)$

$$\begin{aligned}\Delta E &= E_{\text{new}} - E_{\text{old}} = -(S_1' * S_2 * w_{12} + S_1' * S_3 * w_{13} + S_2 * S_3 * w_{23}) + \\ &\quad (S_1 * S_2 * w_{12} + S_1 * S_3 * w_{13} + S_2 * S_3 * w_{23}) \\ &= (S_1 - S_1')(S_2 * w_{12} + S_3 * w_{13}) \\ &= (S_2 * w_{12} + S_3 * w_{13})\end{aligned}$$

$\exp(-\Delta E/T) > \text{threshold}$ **accept**



Boltzmann distribution

- HNN, 3 nodes, the status of each neuron is either 0 or 1
- consider neuron 1, its status S_1 is 1, to determine if it changed to $S_1'(0)$

- Boltzmann distribution: $F(config) \propto \exp(-\frac{E}{kT})$

$$F(new) = \exp(-E_{new}/T)$$

$$F(old) = \exp(-E_{old}/T)$$

- Boltzmann factor

$$F(new)/F(old) = \exp(-\Delta E/T)$$

A probabilistic view

- HNN, 3 nodes, the status of each neuron is either 0 or 1
- consider neuron 1, its status $S1$ is 1, to determine if it changed to $S1'(0)$

$$p(S1=0)=F(\text{new}) = \exp(-E_{\text{new}}/T) \rightarrow E_{\text{new}} = -T \cdot \ln(p(S1=0))$$

$$p(S1=1)=F(\text{old}) = \exp(-E_{\text{old}}/T) \rightarrow E_{\text{old}} = -T \cdot \ln(p(S1=1))$$

$$\Delta E = E_{\text{new}} - E_{\text{old}} = -T \cdot \ln(p(S1=0)) + T \cdot \ln(p(S1=1))$$

$$\frac{\Delta E}{T} = \ln(p(S1 = 1)) - \ln(1 - p(S1 = 1)) = \ln\left(\frac{p(s1 = 1)}{1 - p(s1 = 1)}\right)$$

A probabilistic view – stochastic unit

- HNN, 3 nodes, the status of each neuron is either 0 or 1
- consider neuron 1, its status $S1$ is 1, to determine if it changed to $S1'(0)$

$$\frac{\Delta E}{T} = \ln \left(\frac{p(s1 = 1)}{1 - p(s1 = 1)} \right)$$

$$-\frac{\Delta E}{T} = \ln \left(\frac{1 - p(s1 = 1)}{p(s1 = 1)} \right) = \ln \left(\frac{1}{p(s1 = 1)} - 1 \right)$$

$$\exp \left(-\frac{\Delta E}{T} \right) = \frac{1}{p(s1=1)} - 1 \quad \rightarrow \quad p(s1 = 1) = \frac{1}{1 + \exp \left(-\frac{\Delta E}{T} \right)}$$

sigmoid $\left(-\frac{\Delta E}{T} \right)$

(neuron & Energy)
can be used to
compute prob.

Thermal equilibrium

- Set temperature =1
- Thermal equilibrium is a difficult concept!
 - * • Reaching thermal equilibrium does not mean that the system has settled down into the lowest energy configuration.
 - The thing that settles down is the **probability distribution** over configurations.
 - This settles to the **stationary distribution**.
- A Boltzmann machine is a model which describes data distribution

An analogy

- Imagine a casino in Sentosa that is full of card dealers (we need many more than $52!$ of them).
- We start with all the card packs in standard order and then the dealers all start shuffling their packs.
 - After a few time steps, the king of spades still has a good chance of being next to the queen of spades. The packs have not yet forgotten where they started.
 - After prolonged shuffling, the packs will have forgotten where they started. There will be an equal number of packs in each of the $52!$ possible orders.
 - Once equilibrium has been reached, the number of packs that leave a configuration at each time step will be equal to the number that enter the configuration.
- The only thing wrong with this analogy is that all the configurations have equal energy, so they all end up with the same probability.

5 cards

$$5 \times 4 \times 3 \times 2 \times 1 = 120 \text{ orders}$$

reach equilibrium

120 card packs

S	P(S)
(1 2 3 4 5)	$\frac{1}{120}$
(1 2 3 5 4)	$\frac{1}{120}$
⋮	⋮
(5 4 3 2 1)	$\frac{1}{120}$

→

shuffle

one
more

time

simultaneously

→

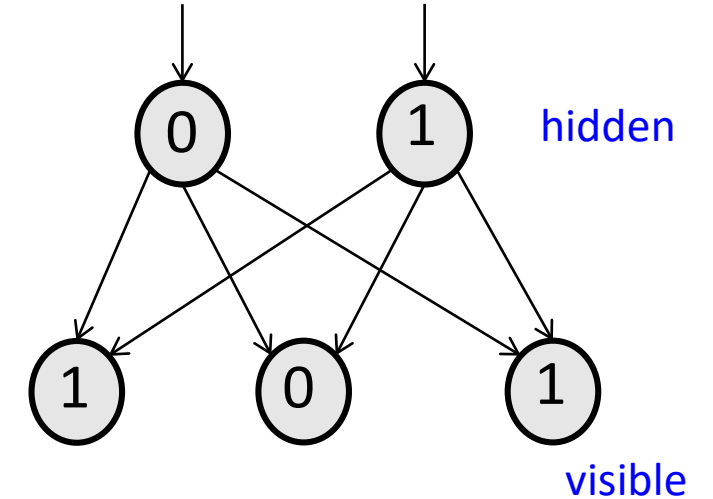
S	P(S)
(1 3 4 5 2)	$\frac{1}{120}$
(1 2 3 4 5)	$\frac{1}{120}$
⋮	⋮
(1 2 3 5 4)	$\frac{1}{120}$



stationary distribution

Boltzmann machine

- A BM has two layers: hidden and visible
- RBM: constraint connectivity,
 - only connect hidden layer and visible layer
- The energy of a joint configuration



$$-E(\mathbf{v}, \mathbf{h}) = \sum_{i \in \text{vis}} v_i b_i + \sum_{k \in \text{hid}} h_k b_k + \sum_{i < j} v_i v_j w_{ij} + \sum_{i, k} v_i h_k w_{ik} + \sum_{k < l} h_k h_l w_{kl}$$

Annotations for the equation:

- $-E(\mathbf{v}, \mathbf{h})$: Energy with configuration \mathbf{v} on the visible units and \mathbf{h} on the hidden units
- $v_i b_i$: binary state of unit i in \mathbf{v} multiplied by bias of unit i
- $h_k b_k$: bias of unit k multiplied by hidden unit state h_k
- $\sum_{i < j} v_i v_j w_{ij}$: indexes every non-identical pair of i and j once (circled in red, labeled RBM)
- $\sum_{i, k} v_i h_k w_{ik}$: weight between visible unit i and hidden unit k (circled in red, labeled RBM)
- $\sum_{k < l} h_k h_l w_{kl}$: weight between hidden units k and l (circled in red, labeled RBM)

Energy \rightarrow probability

- \mathbf{v} : observable features
- \mathbf{h} : cluster/class

\mathbf{v} : (headach = 1, sneeze = 0)

\mathbf{h} : (concussion=1, cold=0)

$$p(\mathbf{v}, \mathbf{h}) = \frac{e^{-E(\mathbf{v}, \mathbf{h})}}{\sum_{\mathbf{u}, \mathbf{g}} e^{-E(\mathbf{u}, \mathbf{g})}}$$

$E(10, 10)$

partition function

$\mathbf{u} \quad \mathbf{g}$

0	0	0	0
0	0	0	1
0	0	1	0
:	:	:	:
1	1	:	1

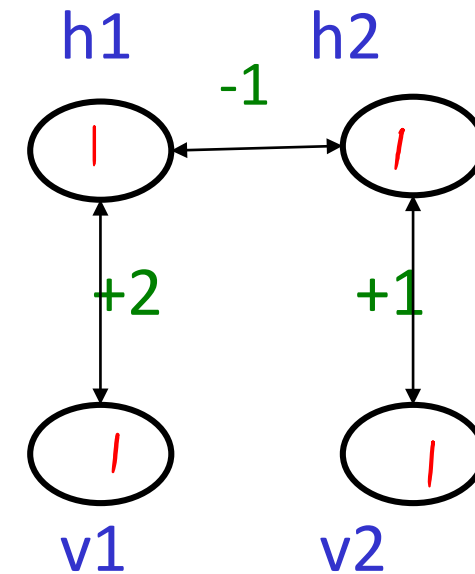
24

$$p(\mathbf{v}) = \frac{\sum_{\mathbf{h}} e^{-E(\mathbf{v}, \mathbf{h})}}{\sum_{\mathbf{u}, \mathbf{g}} e^{-E(\mathbf{u}, \mathbf{g})}}$$

v	h	$-E$	e^{-E}	$p(\mathbf{v}, \mathbf{h})$	$p(\mathbf{v})$
1 1	1 1	2	7.39	.186	0.466 = $\frac{7.39 + 2.72 + 1}{39.7}$
1 1	1 0	2	7.39	.186	
1 1	0 1	1	2.72	.069	
1 1	0 0	0	1	.025	
1 0	1 1	1	2.72	.069	0.305
1 0	1 0	2	7.39	.186	
1 0	0 1	0	1	.025	
1 0	0 0	0	1	.025	
0 1	1 1	0	1	.025	0.144
0 1	1 0	0	1	.025	
0 1	0 1	1	2.72	.069	
0 1	0 0	0	1	.025	
0 0	1 1	-1	0.37	.009	0.084
0 0	1 0	0	1	.025	
0 0	0 1	0	1	.025	
0 0	0 0	0	1	.025	

$$(\sum e^{-E}) = 39.70$$

An example of how weights define a distribution



$$-E = 1 \times 1 \times -1 + 1 \times 1 \times 2 + 1 \times 1 \times 1 + 1 \times 1 \times 1$$

Classify a new vector

- Once the weights are learnt
- Let the visible units clamped to the given new vector
- Change the status for each hidden unit
- Better explanations/classes have low energy/higher probability

MLE with BM

- To maximize the product of the probabilities that the Boltzmann machine assigns to the binary vectors in the training set.

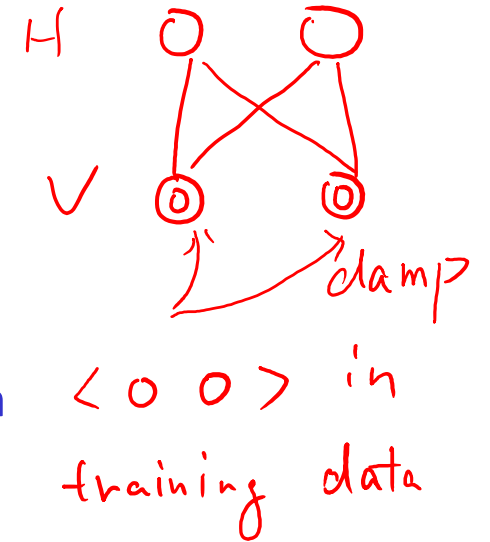
$$\frac{\partial \log p(\mathbf{v})}{\partial w_{ij}} = \langle s_i s_j \rangle_{\mathbf{v}} - \langle s_i s_j \rangle_{model}$$

Derivative of log probability of one training vector, \mathbf{v} under the model.

Expected value of product of states at thermal equilibrium when \mathbf{v} is clamped on the visible units

Expected value of product of states at thermal equilibrium with no clamping

$$\Delta w_{ij} \propto \langle s_i s_j \rangle_{data} - \langle s_i s_j \rangle_{model}$$



An inefficient way to collect the statistics required for learning

Hinton and Sejnowski (1983)

- **Positive phase:** Clamp a data vector on the visible units and set the hidden units to random binary states.

- Update the hidden units one at a time until the network reaches thermal equilibrium at a temperature of 1.
- Sample $\langle s_i s_j \rangle$ for every connected pair of units.
- Repeat for all data vectors in the training set and average.

✓	s_1	s_2	s_3	s_4	H	$\langle s_1 s_3 \rangle$
	0	0	1	1		0
	0	1	1	0		0
	0	0	1	1		0

return $\frac{1}{4}$

- **Negative phase:** Set **all** the units to random binary states.

- Update all the units one at a time until the network reaches thermal equilibrium at a temperature of 1.
- Sample $\langle s_i s_j \rangle$ for every connected pair of units.
- Repeat many times (how many?) and average to get good estimates.

✓	s_1	s_2	s_3	s_4	H	$\langle s_1 s_3 \rangle$
	0	0	1	0		0
	0	0	0	1		0
	0	0	1	1		0
	1	1	0	0		0
	1	0	1	0		1
	1	1	1	0		1

return $\frac{1}{3}$

$\Delta W_{13} = \frac{1}{4} - \frac{1}{3}$

Getting a sample from the model

- Run the machine(Markov chain) until it reaches its stationary distribution (thermal equilibrium at a temperature of 1).
 - Similar to the remembering process in HNN with Simulated Annealing
- The probability of a global configuration is then related to its energy by the Boltzmann distribution

$$p(\mathbf{v}, \mathbf{h}) \propto e^{-E(\mathbf{v}, \mathbf{h})}$$