

#### Restricted Boltzmann Machine

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### Introduction

# Prologue



Boltzmann distribution can be used to determine the distribution of the kinetic energy of for a set of molecules

### Prologue

- Got popular after Netflix competition
- Is a Graphical model
- Used for unsupervised learning
- Has 1 visible and 1 hidden layer
- Involves learning a probability distribution from an original dataset and using it to make inferences about never before seen data

### Basics

# The mystery

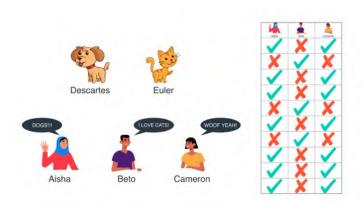


# The mystery

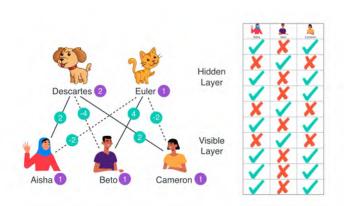




### Solution

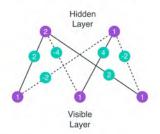


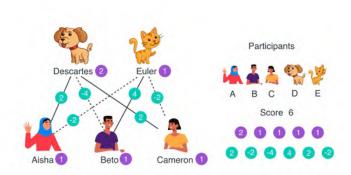
# Weights

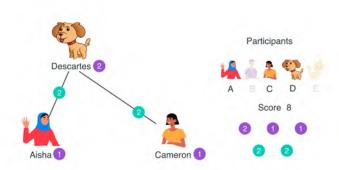


### Model

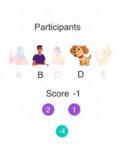
### Restricted Boltzmann Machine (RBM)

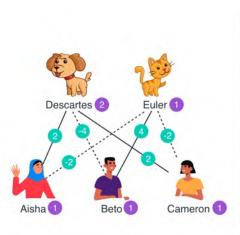




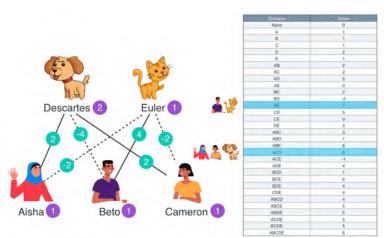


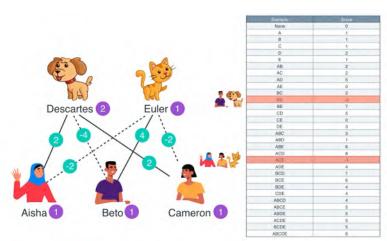






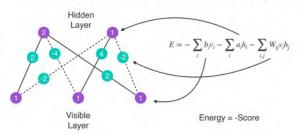
None	0	
A	1	
8	1	
C	1	
D	2	
E	1	
AB	2	
AC	2	
AD		
AE	0	
BC	2	
BD	-2	
BE	7	
CD	.5	
CE	0	
DE	3	
ABC	3	
ABD	1	
ABE	6	
ACD	8	
ACE	-1	
ADE	4	
BCD	1	
BCE	6	
BDE	4	
CDE	-4	
ABCD	4	
ABCE	5	
ABDE	5	
ACDE	5	
BCDE	5	
ABCDE	6	



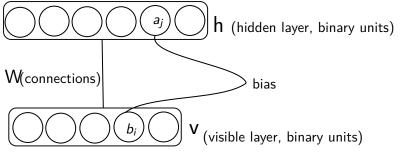


### Model

### Restricted Boltzmann Machine (RBM)



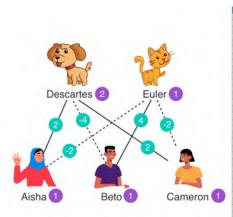
#### Model



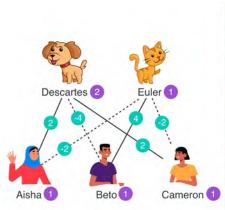
• Energy function:

$$E(v, h) = -h^{T} W v - b^{T} v - a^{T} h$$
  
=  $-\sum_{j} \sum_{i} W_{j,i} h_{j} v_{i} - \sum_{i} b_{i} v_{i} - \sum_{j} a_{j} h_{j}$ 

## Probability and Inference



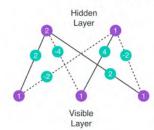
None	0	1	0
A	1.	2.72	0
В	1	2.72	0
C	1	2.72	0
D	2	7.38	0
E	-1	2.72	0
AB	2	7.38	0
AC	2	7.38	0
AD	5	148.41	0.02
AE	0	2.72	0
BC	2	7.38	0
BD	-2	0.14	0
BE	7	1096.63	0.17
CD	5	148.41	0.02
CE	0	1	0
DE	3	20.08	0
ABC	3	20.08	.0
ABD	1	2.72	0
ABE	6	403.43	0.06
ACD	8	2980.96	0.45
ACE	-1	0.37	0
ADE	4	54.6	0
BCD	1	2.72	0
BCE	6	403.43	0.06
BDE	4	54.6	0
CDE	4	54.6	0
ABCD	4	54.6	0.02
ABCE	5	148.41	0.02
ABDE	5	148.41	0.02
ACDE	5	148.41	0.02
BCDE	5	146.41	0.02
ABCDE	6	403.43	0.06



None	0	1	0
A	1	2.72	0
В	1.	2.72	0
c	1	2.72	.0
D	2	7.38	0
E	-1	2.72	0
AB	2	7.38	0
AC	2	7.38	0
AD	5	148.41	0.02
AE	0	2.72	0
BC	2	7.38	0
BD		D.14	.0
BE	7	1096.63	0.17
CD	5	148.41	0.02
CE	0	1	0
DE	3	20.08	0
ABC	3	20.08	.0
ABD	1	2.72	0
ABE	6	403.43	0.06
ACD	8	2950.98	0.45
ACE		0.57	0
ADE	4	54.6	0
BCD	-1	2.72	0
BCE	6	403.43	0.06
BDE	4	54.6	0
CDE	4	54.6	0
ABCD	4	54.6	0.02
ABCE	5	148.41	0.02
ABDE	5	148.41	0.02
ACDE	5	148.41	0.02
BCDE	5	146.41	0.02
ABCDE	6	403.43	0:06

#### Model

# Energy to probability



$$E = -\sum_i b_i v_i - \sum_i a_i h_i - \sum_{i,j} W_{ij} v_i h_j$$

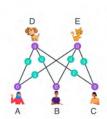
$$p(v,h) = \frac{1}{Z} e^{-E(v,h)} \qquad Z = \sum_{v,h} e^{-E(v,h)}$$

#### Model

$$Z = \sum_{v,h} \exp(-E(v,h))$$
Distribution:  $p(v,h) = \exp(-E(v,h))/Z$ 

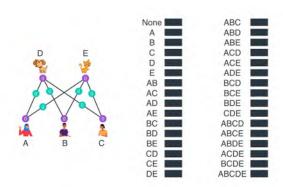
$$= \exp(h^T W v + b^T v + a^T h)/Z$$

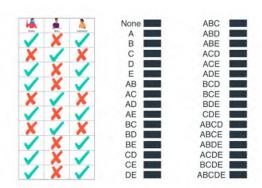
$$= \exp(h^T W v) \exp(b^T v) \exp(a^T h)/Z$$

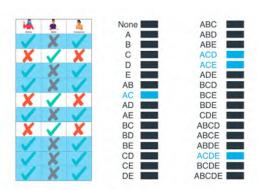


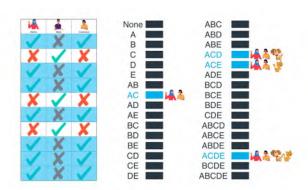
Scenario	Score	Agent	Prubabili
None	0	- 1	1/32
Α	0	1	1/32
В	0	1	1/32
C	0	1	1/32
D	0	1	1/32
E	0	1	1/32
AB	0	1	1/32
AC	0	1	1/32
AD	0	1	1/32
AE	0	1	1/32
BC	0	1	1/32
BD	0	1	1/32
BE	0	1	1/32
CD	0	1	1/32
CE	-0	1	1/32
DE	0	1	1/32

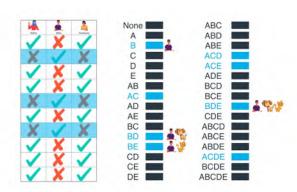
ABC	0	1	1/32
ABD	0	1	1/32
ABE	0	1	1/32
ACD	0	.1	1/32
ACE	0	1	1/32
ADE	0	- 1	1/32
BCD	0	-1	1/32
BCE	0	.1	1/32
BDE	0	1	1/32
CDE	0	1	1/32
ABCD	0	1	1/32
ABCE	0	-1	1/32
ABDE	0	1	1/32
ACDE	0	1	1/32
BCDE	0	1	1/32
ABCDE	0	1	1/32

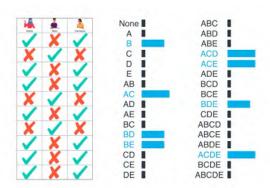


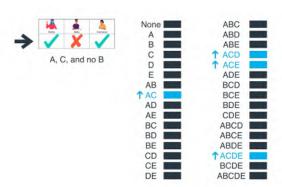


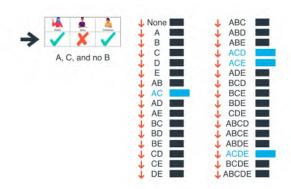


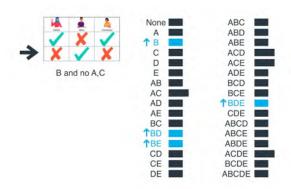


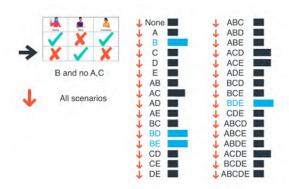


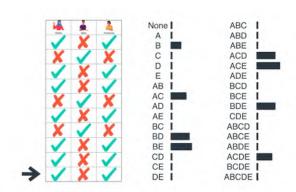




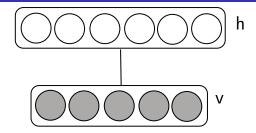








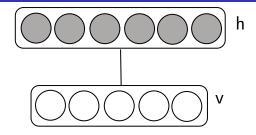
## Conditional distributions



$$p(h|v) = \prod_{j} p(h_{j}|v)$$
$$p(h_{j} = 1|v) = sigm(a_{j} + W_{j}v)$$

W<sub>j</sub> is the jth row of W

# Conditional distributions



$$p(v|h) = \prod_{i} p(v_i|h)$$
$$p(v_i = 1|h) = sigm(b_i + h^T W_i)$$

• W<sub>i</sub> is the ith column of W

$$\begin{split} \rho(h|v) &= \rho(v,h) / \sum_{h'} \rho(v,h') \\ &= \frac{\exp(h^T W.v) \exp(b^T v) \exp(a^T h) / Z}{\sum_{h' \in \{0,1\}^H} \exp(h'^T W v) \exp(b^T v) \exp(a^T h') / Z} \\ &= \frac{\exp(\sum_j h_j W_j.v + a_j h_j)}{\sum_{h'_1 \in \{0,1\}} \dots \sum_{h'_H \in \{0,1\}} \exp(\sum_j h'_j W_j.v + a_j h'_j)} \\ &= \frac{\prod_j \exp(h_j W_j.v + a_j h_j)}{\sum_{h'_1 \in \{0,1\}} \dots \sum_{h'_H \in \{0,1\}} \prod_j \exp(h'_j W_j.v + a_j h'_j)} \\ &= \frac{\prod_j \exp(h_j W_j.v + a_j h_j)}{(\sum_{h'_1 \in \{0,1\}} \exp(h'_1 W_1.v + a_1 h'_1)) \dots (\sum_{h'_H \in \{0,1\}} \exp(h'_H W_H.v + a_H h'_H))} \end{split}$$

$$= \frac{\prod_{j} \exp(h_{j}W_{j}.v + a_{j}h_{j})}{\prod_{j}(\sum_{h'_{j\in\{0,1\}}} \exp(h'_{j}W_{j}.v + a_{j}h'_{j})}$$

$$= \frac{\prod_{j} \exp(h_{j}W_{j}.v + a_{j}h_{j})}{\prod_{j}(1 + \exp(W_{j}.v + a_{j}h_{j}))}$$

$$= \prod_{j} \left[\frac{\exp(h_{j}W_{j}.v + a_{j}h_{j})}{1 + \exp(W_{j}.v + a_{j})}\right]$$

$$= \prod_{j} p(h_{j}|v)$$

$$p(h_{j} = 1|v) = \frac{\exp(a_{j} + W_{j}.v)}{1 + \exp(a_{j} + W_{j}.v)}$$
$$= \frac{1}{1 + \exp(-a_{j} - W_{j}.v)}$$
$$= sigm(a_{j} + W_{j}.v)$$

# Free energy

• 
$$p(v) = \sum_{h \in \{0,1\}^H} p(v,h) = \sum_{h \in \{0,1\}^H} \exp(-E(v,h))/Z$$

• 
$$p(v) = \exp(b^T v + \sum_{i=1}^{H} \log(1 + \exp(a_i + W_{j.}v)))/Z$$

$$p(v) = \exp(-F(v))/Z$$

$$p(v) = \sum_{h \in \{0,1\}^H} \exp(h^T W v + b^T v + a^T h)/Z$$
  
=  $\exp(b^T v) \sum_{h_1 \in \{0,1\}} \cdots \sum_{h_H \in \{0,1\}} \exp(\sum_j h_j W_j v + a_j h_j)/Z$ 

$$= \exp(b^{T}v)(\sum_{h_{1} \in \{0,1\}} \exp(h_{1}W_{1}v + a_{1}h_{1})) \dots (\sum_{h_{H} \in \{0,1\}} \exp(h_{H}W_{H}v + a_{H}h_{H}))/Z$$

$$= \exp(b^{T}v)(1 + \exp(W_{1}v + a_{1})) \dots (1 + \exp(W_{H}v + a_{H}))/Z$$

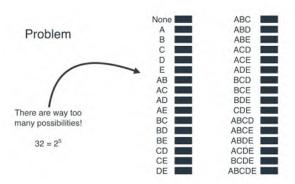
$$= \exp(b^{T}v) \exp(\log(1 + \exp(W_{1}v + a_{1}))) \dots \exp(\log(1 + \exp(W_{H}v + a_{H})))/Z$$

$$= \exp(b^{T}v + \sum_{i=1}^{H} \log(1 + \exp(W_{i}v + a_{i})))/Z$$

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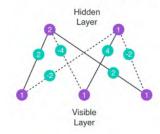
# Some Details

### Problem

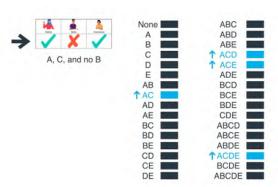


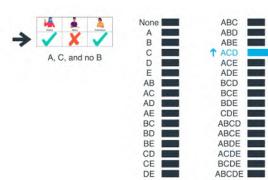
# Model

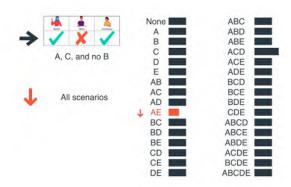
## Partition function is intractable

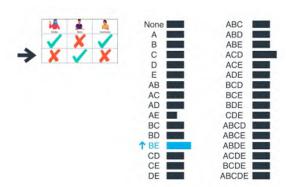


$$p(v,h) = \frac{1}{Z}e^{-E(v,h)} \qquad Z = \sum_{v,h} e^{-E(v,h)}$$
 Intractable

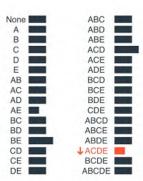


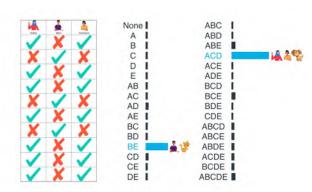


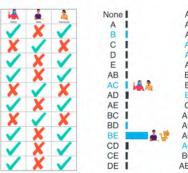


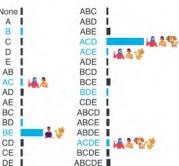




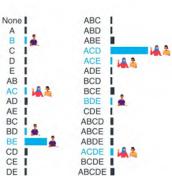


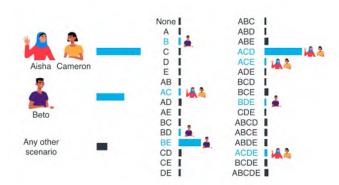


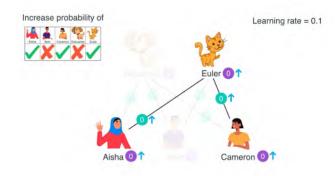


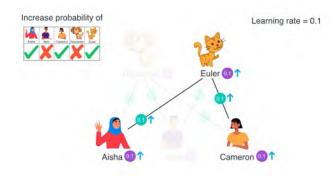


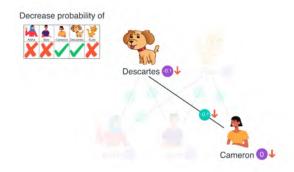


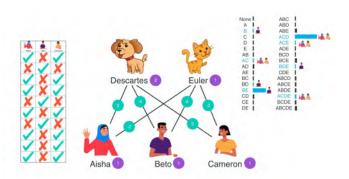


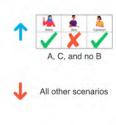


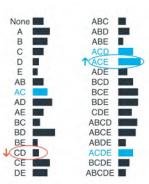


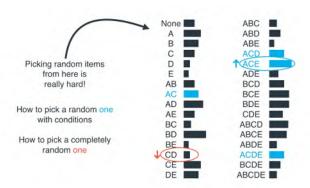




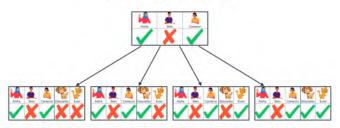








# Gibbs Sampling











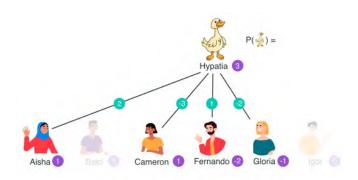


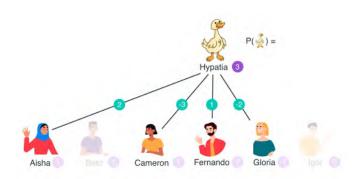


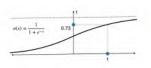














$$P(\frac{1}{6}) = \sigma(1)$$
$$= 0.73$$



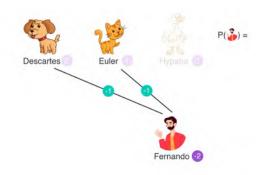


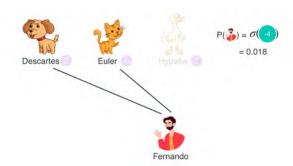




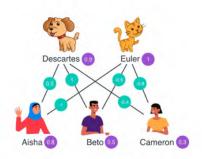


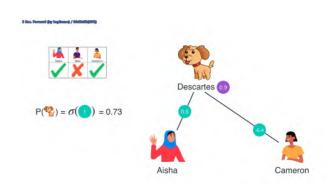


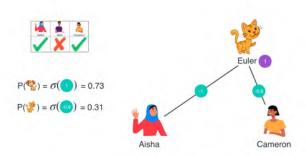










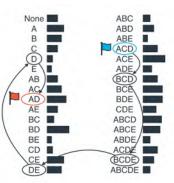


## How to Pick

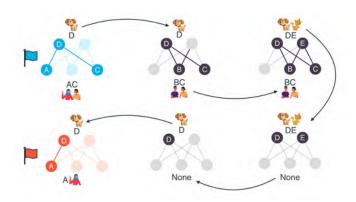
### Gibbs Sampling



How to pick a totally random sample from this distribution



# How to Pick



# How to Pick

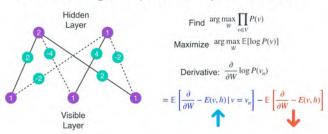
# Increase scores



# Contrastive Divergence

# Model

# Maximizing the probability of the data



# Traning objective

Minimize the average negative log-likelihood (NLL)

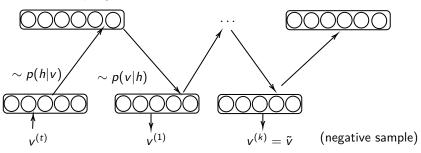
$$\frac{1}{T}\sum_{t}-\log p(v^{(t)})$$

We'd like to proceed by stochastic gradient descent

$$\frac{\partial -\log p(v^{(t)})}{\partial \theta} = \mathbb{E}_h[\frac{\partial}{\partial \theta} - \mathbb{E}(v^{(t)}, h)|v^{(t)}] - \mathbb{E}_{v, h}[\frac{\partial}{\partial \theta} \mathbb{E}(v, h)]$$

### Idea

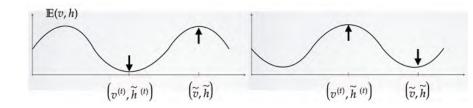
- ullet replace the expectation by a point estimate at  $ilde{v}$
- ullet obtain the point  $\tilde{v}$  by Gibbs sampling
- start sampling chain at  $v^{(t)}$



# Approximation

• 
$$\mathbb{E}_h[\frac{\partial}{\partial \theta}\mathbb{E}(v^{(t)},h)|v^{(t)}] = \frac{\partial}{\partial \theta}\mathbb{E}(v^{(t)},\tilde{h}^{(t)})$$

• 
$$\mathbb{E}_{v,h}[\frac{\partial}{\partial \theta}\mathbb{E}(v,h)] = \frac{\partial}{\partial \theta}\mathbb{E}(\tilde{v},\tilde{h})$$



## Inference

$$ullet$$
  $\frac{\partial}{\partial heta} \mathbb{E}(v,h)$  for  $heta = W_{ji}$ 

$$\bullet \ \frac{\partial}{\partial W_{ji}}\mathbb{E}(v,h) = -h_j v_i$$

• 
$$\nabla_W \mathbb{E}(v,h) = -hv^T$$

• 
$$\mathbb{E}_h[\frac{\partial}{\partial \theta}\mathbb{E}(v,h)|v]$$
 for  $\theta = W_{jj}$ 

• 
$$\mathbb{E}_h[\frac{\partial}{\partial \theta}\mathbb{E}(v,h)|v] = \mathbb{E}_h[-h_iv_i] = -v_ip(h_i=1|v)$$

• 
$$\mathbb{E}_h[\nabla_W \mathbb{E}_h(v,h)|v] = -h(v)v^T$$

## Inference

Given  $v^{(t)}$  and  $\tilde{v}$  the learning rule for  $\theta = W$  becomes

• 
$$W_{new} = W - \alpha(\nabla_W - \log p(v^{(t)}))$$

• 
$$W_{new} = W - \alpha(\mathbb{E}_h[\nabla_W \mathbb{E}(v^{(t)}, h)|v^{(t)}] - \mathbb{E}_{v,h}[\nabla_W \mathbb{E}(v, h)])$$

• 
$$W_{new} = W - \alpha(\mathbb{E}_h[\nabla_W \mathbb{E}(v^{(t)}, h)|v^{(t)}] - \mathbb{E}_v[\nabla_W \mathbb{E}(\tilde{v}, h)|\tilde{v}])$$

• 
$$W_{new} = W + \alpha (h(v^{(t)})v^{(t)^T} - h(\tilde{v})\tilde{v}^T)$$

# Inference

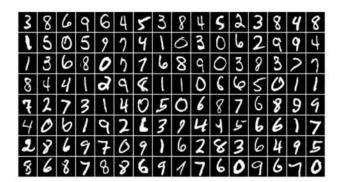
• 
$$W_{new} = W + \alpha (h(v^{(t)})v^{(t)^T} - h(\tilde{v})\tilde{v}^T)$$

• 
$$a_{new} = a + \alpha(h(v^{(t)}) - h(\tilde{v}))$$

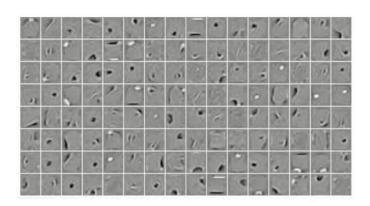
• 
$$b_{new} = b + \alpha (v^{(t)} - \tilde{v})$$

# **Application**

# **MNIST**



# Filter



# **Extensions**

- k=1 Gibbs sampling
- Persistent CD
- Debugging
- RBM for unbounded reals
- Boltzmann machine & semi-restricted Boltzmann machine

# Thank you for your time



# Refrences

- A Practical Guide to Training Restricted Boltzmann Machines: +
- Examples are from Luis Serrano: +
- Neural networks class Université de Sherbrooke +