Hyperbolic Restricted Boltzmann Machines for Hierarchical Learning

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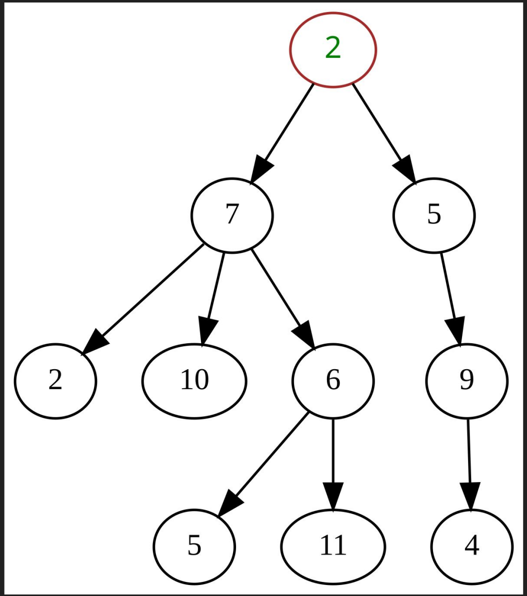
Overview

- Problem:
  - Traditional RBMs use Euclidean geometry, which distorts hierarchical/tree-like data.
  - Key Gap: Can hyperbolic geometry improve RBMs for hierarchical structures?
- Solution:
  - A **Hyperbolic RBM** with adjusted energy function and sampling.
- Impact:
  - Better unsupervised learning for NLP, biology, or knowledge graphs.

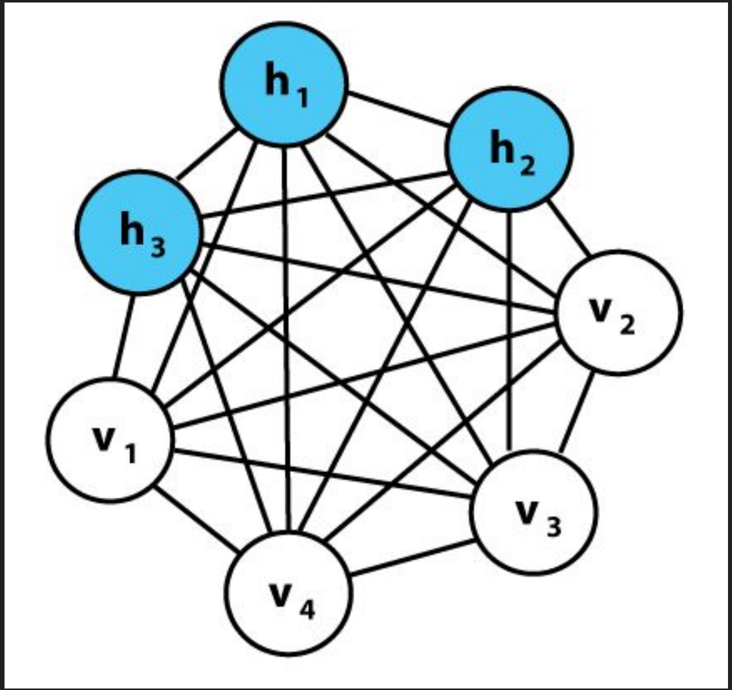


Literature Review

- Masaki Kobayashi
  - Researches the use of non-Euclidean geometry in Hopfield Neural Networks (complex, hyperbolic, quaternion, rotor, etc.)
- John J. Hopfield
  - Invented the Hopfield Neural Network (1982)
  - 2024 Nobel Prize in Physics
- Geoffrey Hinton
  - Invented the Boltzmann Machine (1983-1985)
  - 2024 Nobel Prize in Physics

What is a Boltzmann Machine

- Stochastic, generative neural networks that learn patterns by minimizing an energy function
- Inspired by statistical mechanics (Boltzmann distribution)
- Why they matter:
  - Foundation for energy-based models, latent variable learning, and modern generative AI.

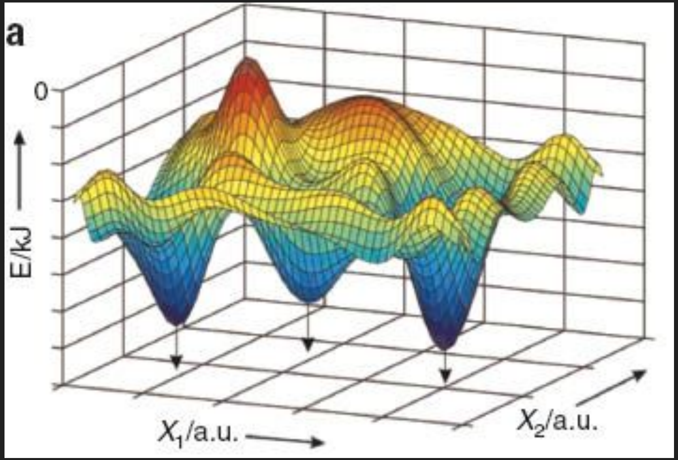


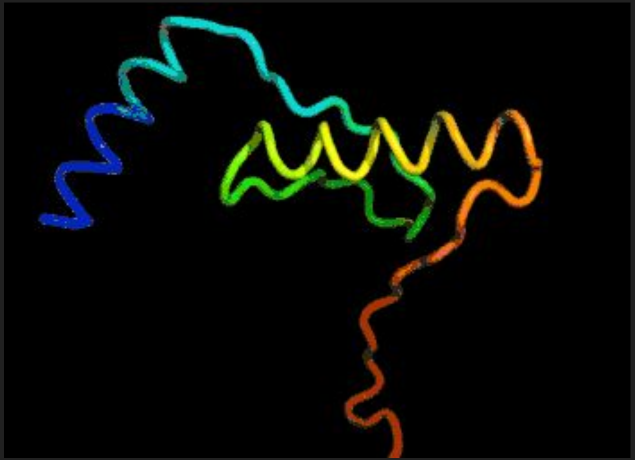
Energy Computation

$$E(\mathbf{v}, \mathbf{h}) = -\mathbf{v}^T W \mathbf{h} - \mathbf{a}^T \mathbf{v} - \mathbf{b}^T \mathbf{h}$$

Measures the "goodness" of a configuration (lower energy = higher probability)

Learning involves adjusting weights to reduce energy for training data



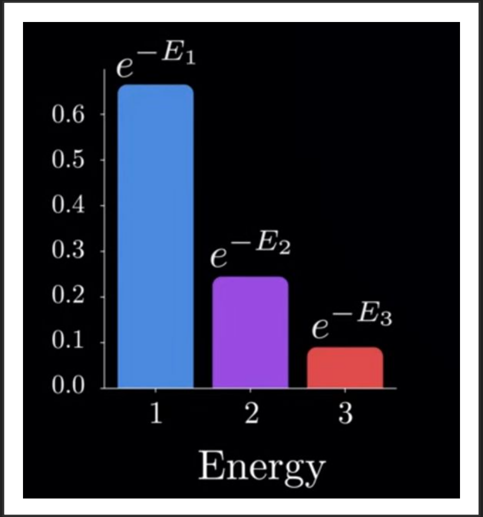


Energy Computation

- The energy function is used to compute the **probability distribution** over all possible configurations of the units.
- Specifically, the probability of a configuration is given by the Boltzmann distribution:

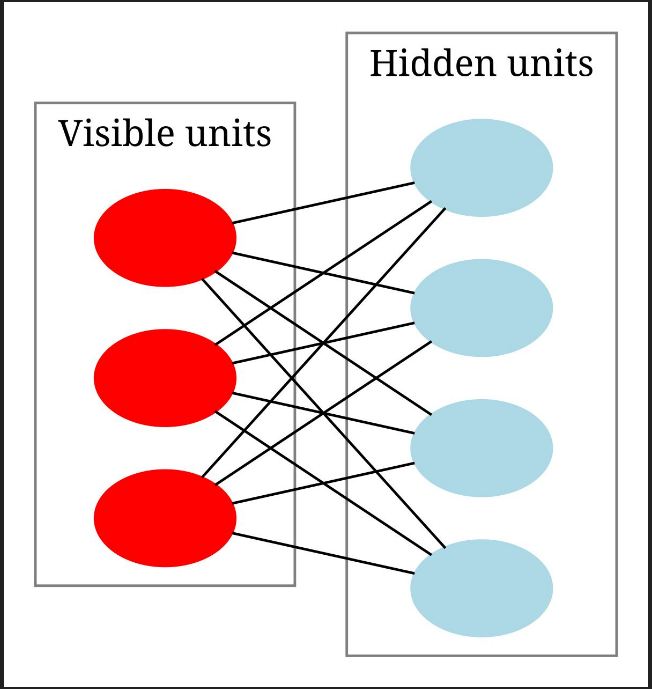
$$p(\mathbf{v}, \mathbf{h}) = \frac{\exp(-E(\mathbf{v}, \mathbf{h}))}{Z}$$

(*Z* is a normalizing function, the sum of all possible state probabilities)



Restricted Boltzmann Machines

- Structure:
  - A simplified Boltzmann Machine with restricted architecture
  - No intra-layer connections: only visible-to-hidden links
- Training:
  - Contrastive Divergence (CD-k): Approximate gradient using Gibbs sampling (fast, but biased)



Boltzmann Machine Simple Example

Let's say you have a dataset of movie preferences for three people. Each person rates whether they like (1) or dislike (0) two movies.

The dataset consists of the following vectors:

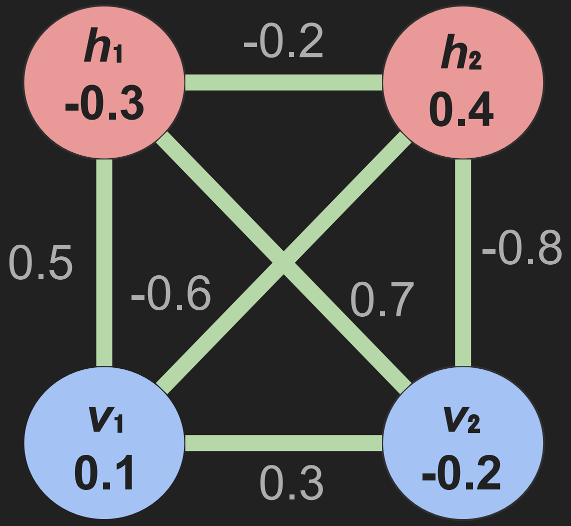
- $x_1 = [1, 0]$ (Person 1 likes Movie A and dislikes Movie B)
- $x_2 = [0, 1]$ (Person 2 dislikes Movie A and likes Movie B)
- $x_3 = [1, 1]$ (Person 3 likes Movie A and Movie B)

Our goal is to train a Boltzmann Machine to learn the underlying patterns in this dataset.

Boltzmann Machine Simple Example

We create the architecture to represent this data:

- Visible units represent the movie preferences (movie A/B)
- Hidden units capture latent (unmeasured) features
- Weights connect units (pos/neg relationship between units)
- Visible and hidden units have biases that measure individual probability of being on or off



Initial values are chosen randomly or from domain knowledge

Restricted Boltzmann Machine Simple Example

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- Visible units represent the movie preferences (movie A/B)
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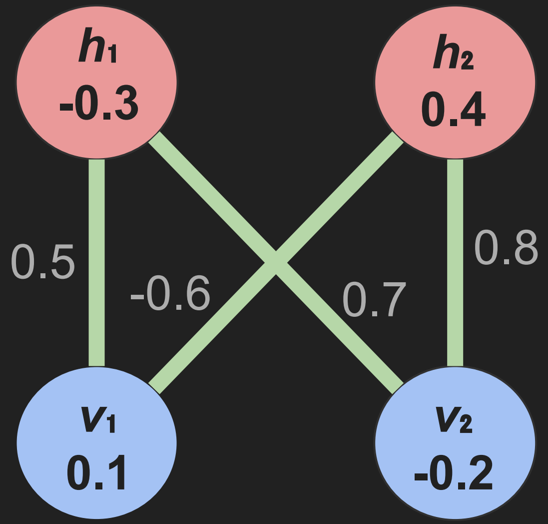


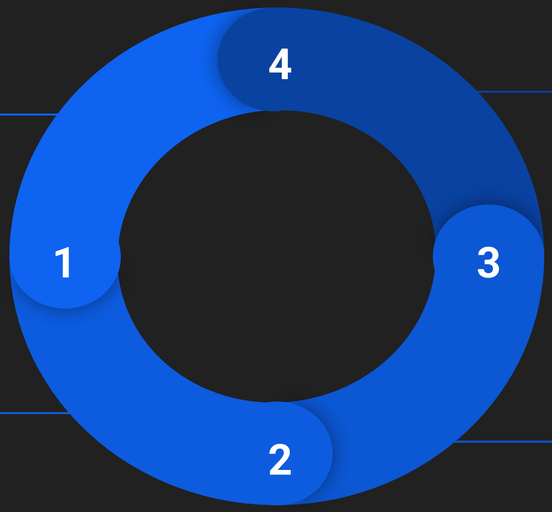
Initial values are chosen randomly or from domain knowledge

Training RBMs: Steps

0. Initialize weights and biases

1. Forward Pass (Visible → Hidden)

2. Reconstruct Input (Hidden → Visible)



4. Update weights and biases

3. Forward Pass Again (Reconstructed Visible → Hidden)

5. Repeat steps 1-4 for all data points and multiple epochs until convergence

Training RBMs: Approximation

Theoretical:

- Goal: Maximize the likelihood of the training data under the RBM's energy-based model
- Problem: Requires the partition function Z, which sums up all possible configurations of the model. Too many calculations for large models.

Contrastive Divergence:

- Solution: Approximate the gradient by running Gibbs Sampling and stopping before equilibrium
- Why it works: Just a few steps of Gibbs tells us the direction of gradient needed to reduce energy.

Step 1: Forward Pass

Sampling is used to infer hidden states given visible states

$$p(h_j = 1|\mathbf{v}) = \sigma\left(b_j + \sum_i v_i w_{ij}\right)$$

$$\sigma(x) = \frac{1}{1+e^{-x}}$$

Sampling for v = [1, 0] (person 1):

h1: $\sigma(-0.3 + 1 \cdot 0.5 + 0 \cdot 0.7) = \sigma(0.2) \approx 0.5498$. Sampled $h_1 = 1$.

h2: $\sigma(0.4 + 1 \cdot (-0.6) + 0 \cdot (-0.8)) = \sigma(-0.2) \approx 0.4502$. Sampled $h_2 = 0$.

Therefore, our hidden activation is h = [1, 0] for this visible state.

Step 2: Reconstruct Input

Now, we sample visible nodes (input) using *h* = [1, 0] from previous step:

$$P(v_i = 1|h) = \sigma(a_i + \textstyle\sum_j h_j W_{ij})$$

v1: $\sigma(0.1 + 1 \cdot 0.5 + 0 \cdot (-0.6)) = \sigma(0.6) \approx 0.6457$. Sampled $v_1' = 1$.

v2: $\sigma(-0.2 + 1 \cdot 0.7 + 0 \cdot (-0.8)) = \sigma(0.5) \approx 0.6225$. Sampled $v_2' = 1$.

Therefore, our reconstructed input is *v'* = [1, 1].

Step 3: Forward Pass (again)

$$p(h_j = 1|\mathbf{v}) = \sigma\left(b_j + \sum_i v_i w_{ij}\right)$$

$$\sigma(x) = \frac{1}{1+e^{-x}}$$

Sampling for *v'* = [1, 1]:

h1': $\sigma(-0.3 + 1 \cdot 0.5 + 1 \cdot 0.7) = \sigma(0.9) \approx 0.7109$. Sampled $h'_1 = 1$.

h2': $\sigma(0.4 + 1 \cdot (-0.6) + 1 \cdot (-0.8)) = \sigma(-1.0) \approx 0.2689$. Sampled $h'_2 = 0$.

Therefore, our reconstructed hidden activation is *h'* = [1, 0].

Step 4: Update Parameters

Goal: Adjust weights and biases to minimize difference between *v* and *v'*

$$\Delta W = \epsilon \left(\mathbf{v}^T\mathbf{h} - \mathbf{v}'^T\mathbf{h}'\right)$$

$$= \epsilon \left(\begin{bmatrix} 1 \\ 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \end{bmatrix} - \begin{bmatrix} 1 \\ 1 \end{bmatrix} \begin{bmatrix} 1 & 0 \end{bmatrix} \right)$$

$$= 0.1 \left(\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} - \begin{bmatrix} 1 & 0 \\ 1 & 0 \end{bmatrix} \right)$$

$$= \begin{bmatrix} 0 & 0 \\ -0.1 & 0 \end{bmatrix}$$

$$\Delta \mathbf{a} = \epsilon(\mathbf{v} - \mathbf{v}')$$

$$= 0.1 \left(\begin{bmatrix} 1 & 0 \end{bmatrix} - \begin{bmatrix} 1 & 1 \end{bmatrix} \right)$$

$$= \begin{bmatrix} 0 & -0.1 \end{bmatrix}$$

$$\Delta \mathbf{b} = \epsilon(\mathbf{h} - \mathbf{h}')$$

$$= 0.1 \left(\begin{bmatrix} 1 & 0 \end{bmatrix} - \begin{bmatrix} 1 & 0 \end{bmatrix} \right)$$

$$= \begin{bmatrix} 0 & 0 \end{bmatrix}$$

Step 4: Update Parameters

Now, we can update the original parameters

$$W_{\text{new}} = W + \Delta W = \begin{bmatrix} 0.5 & -0.6 \\ 0.7 & -0.8 \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ -0.1 & 0 \end{bmatrix} = \begin{bmatrix} 0.5 & -0.6 \\ 0.6 & -0.8 \end{bmatrix}$$

$$\mathbf{a}_{\text{new}} = \mathbf{a} + \Delta \mathbf{a} = \begin{bmatrix} 0.1 & -0.2 \end{bmatrix} + \begin{bmatrix} 0 & -0.1 \end{bmatrix} = \begin{bmatrix} 0.1 & -0.3 \end{bmatrix}$$

$$\mathbf{b}_{\text{new}} = \mathbf{b} + \Delta \mathbf{b} = \begin{bmatrix} -0.3 & 0.4 \end{bmatrix} + \begin{bmatrix} 0 & 0 \end{bmatrix} = \begin{bmatrix} -0.3 & 0.4 \end{bmatrix} \quad \text{(no change)}$$

Step 5: Repeat steps 1-4 for all data points and multiple epochs until convergence

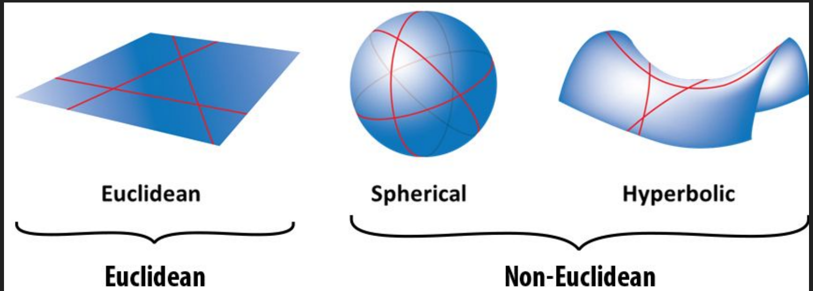
Legacy in Modern Machine Learning

- Deep Belief Networks (DBNs):
  - Stacked RBMs → Unsupervised pre-training → Fine-tuning with backprop
  - Pioneered the "deep learning revolution" (2006–2012)
- Connections to Modern Models:
  - Energy-based models (e.g., VAEs, diffusion models)
  - Stochastic units in GANs/VAEs vs. BM’s Gibbs sampling
- Why They Faded:
  - Computationally expensive vs. backpropagation-friendly architectures (CNNs, Transformers)

Key Takeaway: Understanding Boltzmann Machines reveals the DNA of modern generative AI

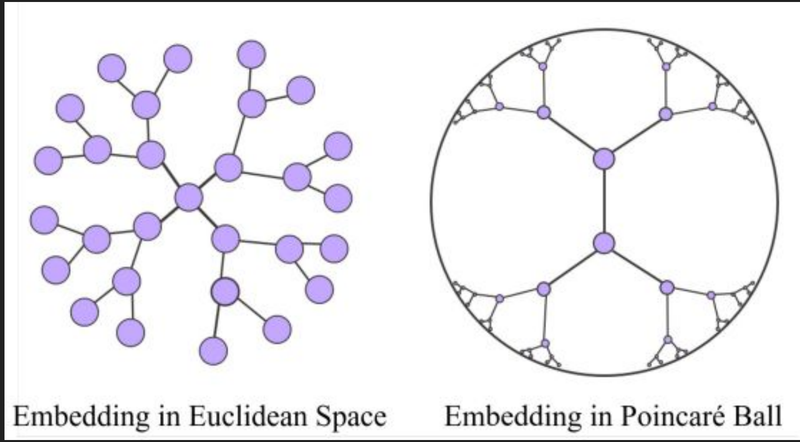
A Primer on Hyperbolic Geometry

- A non-Euclidean geometry with constant negative curvature (like a saddle or pringle shape).
- Contrast with:
  - Euclidean (flat) space: Zero curvature.
  - Spherical geometry: Positive curvature (like a sphere).
- In hyperbolic space, distances grow exponentially as you move outward.



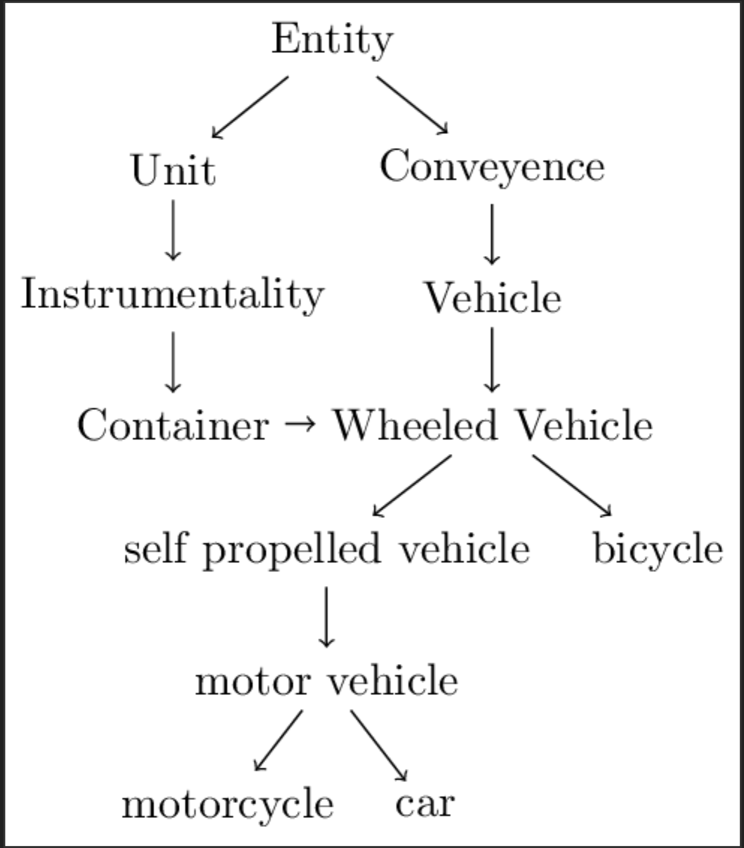
Hyperbolic Models: A Tool for Hierarchical Data

- Represent data points in hyperbolic space (e.g., Poincaré ball)
- Distance between points: $d(x,y) = \operatorname{arcosh}\left(1 + 2\frac{\|x-y\|^2}{(1-\|x\|^2)(1-\|y\|^2)}\right)$
- Efficient representation of hierarchies (fewer dimensions, lower distortion).



WordNet Hierarchy

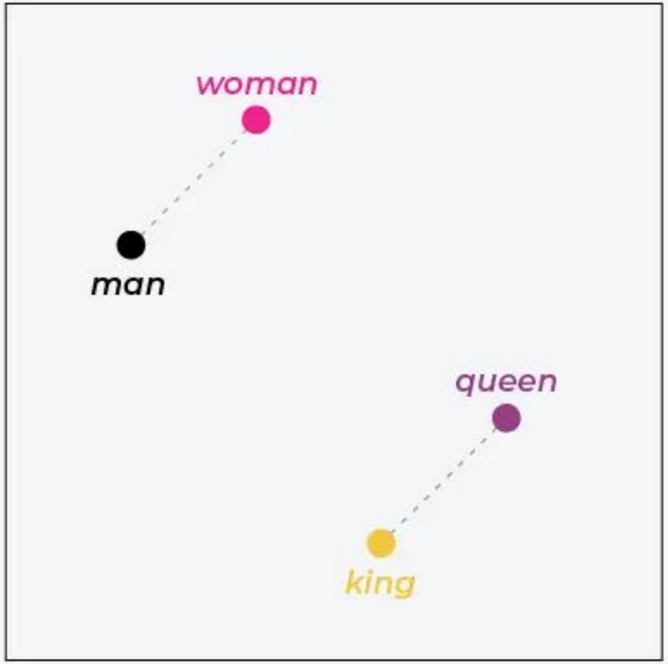
- A lexical database where nouns are organized in a hierarchical taxonomy (e.g., "animal" → "mammal" → "dog").
- Tree-like structure with clear parent-child relationships.
- Access: nltk.corpus.wordnet



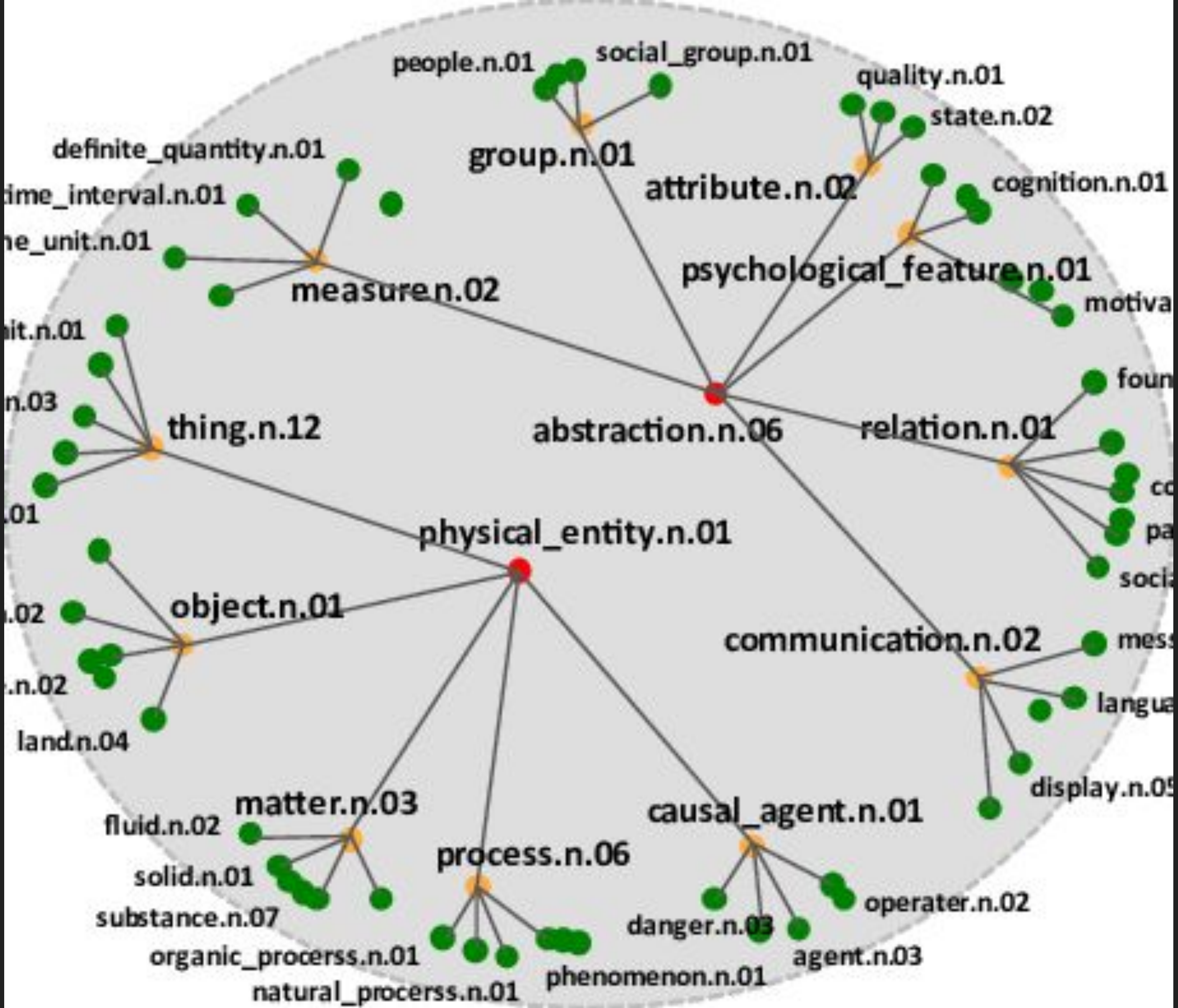
word	living being	feline	human	gender	royalty	verb	plural
man	0.6	-0.2	0.8	0.9	-0.1	-0.9	-0.7
woman	0.7	0.3	0.8	-0.7	0.1	-0.5	-0.4
king	0.5	-0.4	0.7	0.8	0.9	-0.7	-0.6
queen	0.8	-0.1	0.8	-0.9	0.8	-0.5	-0.9

word

Word embedding



Visualization of word embedding


people.n.01
social_group.n.01
quality.n.01
state.n.02
group.n.01
definite_quantity.n.01
attribute.n.02
cognition.n.01
ime_interval.n.01
ne_unit.n.01
psychological_feature.n.01
measure.n.02
motiva
it.n.01
foun
n.03
thing.n.12
abstraction.n.06
relation.n.01
co
.01
pa
physical_entity.n.01
socia
object.n.01
.n.02
communication.n.02
mess
.n.02
langua
land.n.04
display.n.05
matter.n.03
causal_agent.n.01
fluid.n.02
process.n.06
solid.n.01
operater.n.02
substance.n.07
danger.n.03
organic_procerss.n.01
agent.n.03
phenomenon.n.01
natural_procerss.n.01

Model Design: Energy Function

Euclidean RBM:

$$E(\mathbf{v}, \mathbf{h}) = -\mathbf{v}^T W \mathbf{h} - \mathbf{a}^T \mathbf{v} - \mathbf{b}^T \mathbf{h}$$

- $\mathbf{v}$: Visible units.
- $\mathbf{h}$: Hidden units.
- W: Weight matrix.
- $\mathbf{a}, \mathbf{b}$: Bias vectors.

Hyperbolic RBM:

$$E(\mathbf{v}, \mathbf{h}) = -\beta \cdot d_{\mathbb{H}}(\mathbf{v}, W \otimes \mathbf{h})^2 - \mathbf{a}^T \otimes \mathbf{v} - \mathbf{b}^T \otimes \mathbf{h}$$

- $d_{\mathbb{H}}$: Hyperbolic distance in the Poincaré ball.
- $\otimes$: Lorentzian inner product (analog of dot product).
- β: Scaling factor for curvature.

Model Design: Sampling Methods

Euclidean RBM:

- Gibbs Sampling: Sample $h|v$ and $v|h$ using logistic activation
- Markov chain typically converges quickly

$$p(h_j = 1|\mathbf{v}) = \sigma\left(b_j + \sum_i v_i w_{ij}\right)$$

$$p(v_i = 1|\mathbf{h}) = \sigma\left(a_i + \sum_j h_j w_{ij}\right)$$

Hyperbolic RBM:

- Gibbs Sampling: Sample h|v and v|h using hyperbolic probabilities
- Markov chain may take longer to converge due to curvature

$$p(h_j = 1|\mathbf{v}) = \sigma\left(\mathrm{logit}_{\mathbb{H}}(b_j \oplus \sum_i v_i \otimes w_{ij})\right)$$

$$p(v_i = 1|\mathbf{h}) = \sigma\left(\mathrm{logit}_{\mathbb{H}}(a_i \oplus \sum_j h_j \otimes w_{ij})\right)$$

- $\oplus$: Möbius addition.
- $\mathrm{logit}_{\mathbb{H}}$: Hyperbolic logit function.

Model Design: Training

Euclidean RBM:

- Update weights and biases using gradient ascent:

$$\Delta w_{ij} = \epsilon \left(\langle v_i h_j \rangle_{\text{data}} - \langle v_i h_j \rangle_{\text{model}} \right)$$

ϵ: Learning rate.

- Key Properties:
  - Gradients are computed using standard backpropagation.
  - Optimization is stable and efficient.

Hyperbolic RBM:

- Update weights and biases using Riemannian gradient ascent:

$$\Delta w_{ij} = \epsilon \cdot \mathrm{proj}_{\mathbb{H}} \left(\langle v_i h_j \rangle_{\text{data}} - \langle v_i h_j \rangle_{\text{model}} \right)$$

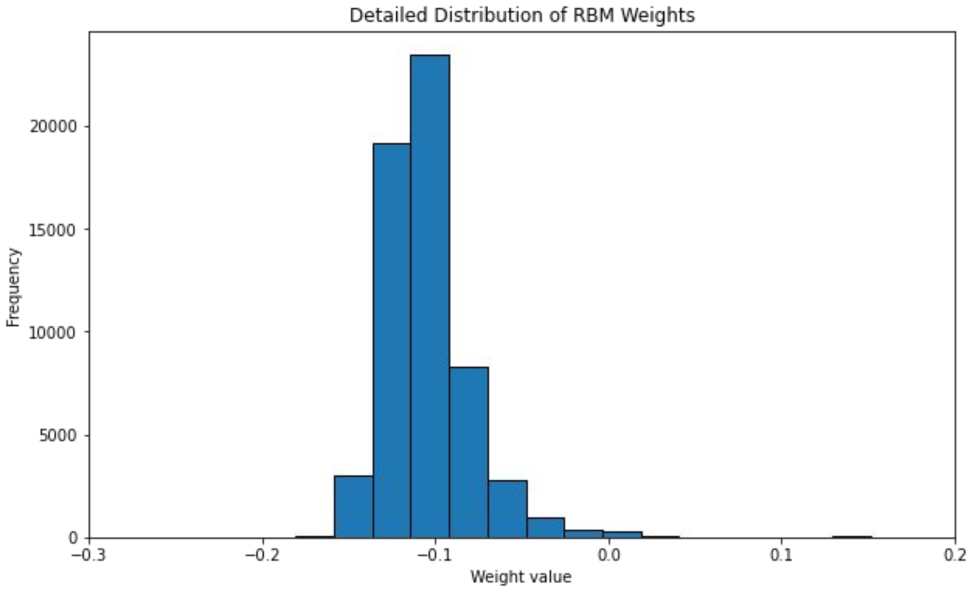
$\mathrm{proj}_{\mathbb{H}}$: Projection onto the hyperbolic manifold.

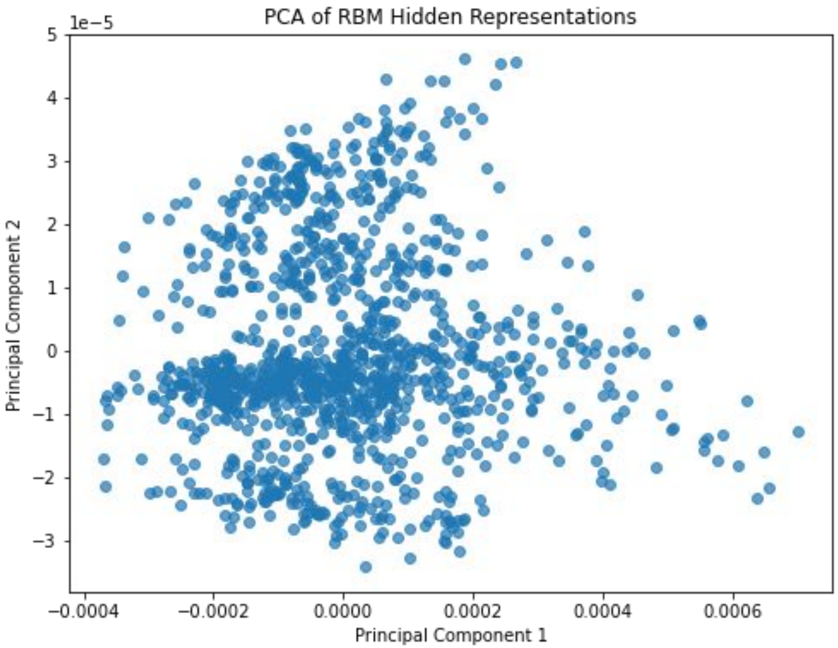
- Key Properties:
  - Gradients must respect the hyperbolic geometry (e.g., Riemannian optimization).
  - Optimization is more challenging due to curvature and numerical instability.

Implementation

Jupyter notebook, nltk wordnet, numpy, sklearn (for BernoulliRBM), matplotlib, networkx (for visualization)

I ran both models on the 1.2k synset “mammal” tree





Results

<u>Euclidean</u>

50 hidden layers, 50 epochs

```
Chosen Sample Node:
pug.n.01

Original active synsets:
['canine.n.02', 'carnivore.n.01', 'dog.n.01', 'mammal.n.01', 'placental.n.0
1', 'pug.n.01']

Reconstructed active synsets:
['ape.n.01', 'equine.n.01', 'even-toed_ungulate.n.01', 'horse.n.01', 'mamma
l.n.01', 'odd-toed_ungulate.n.01', 'placental.n.01']
```

```
Reconstruction error (mean absolute difference): 0.0077
```

```
Precision=0.286, Recall=0.333, F1=0.308
```

<u>Hyperbolic</u>

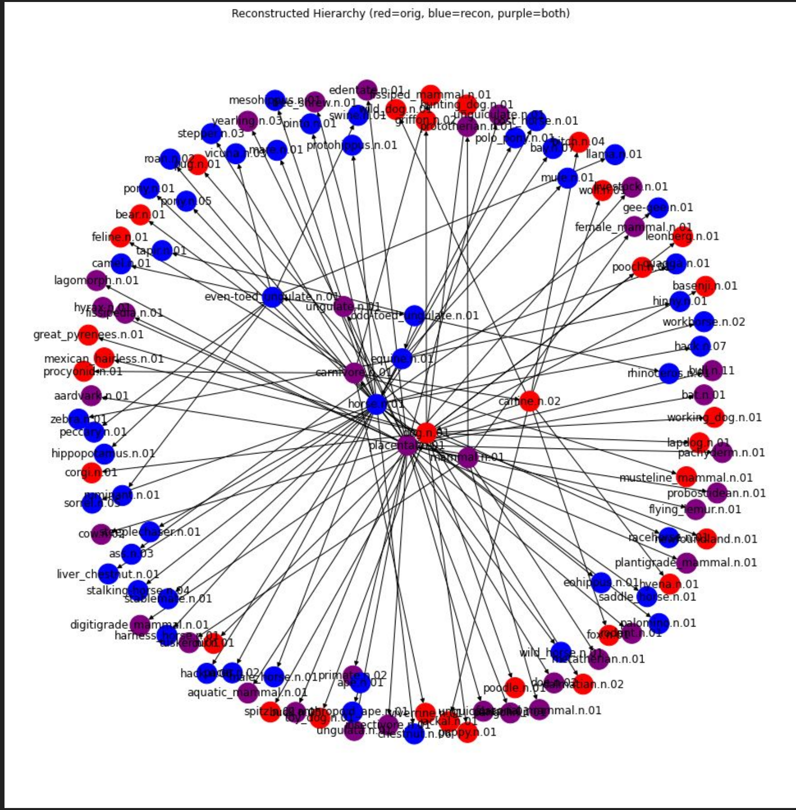
50 hidden layers, 3 epochs (~60 min)

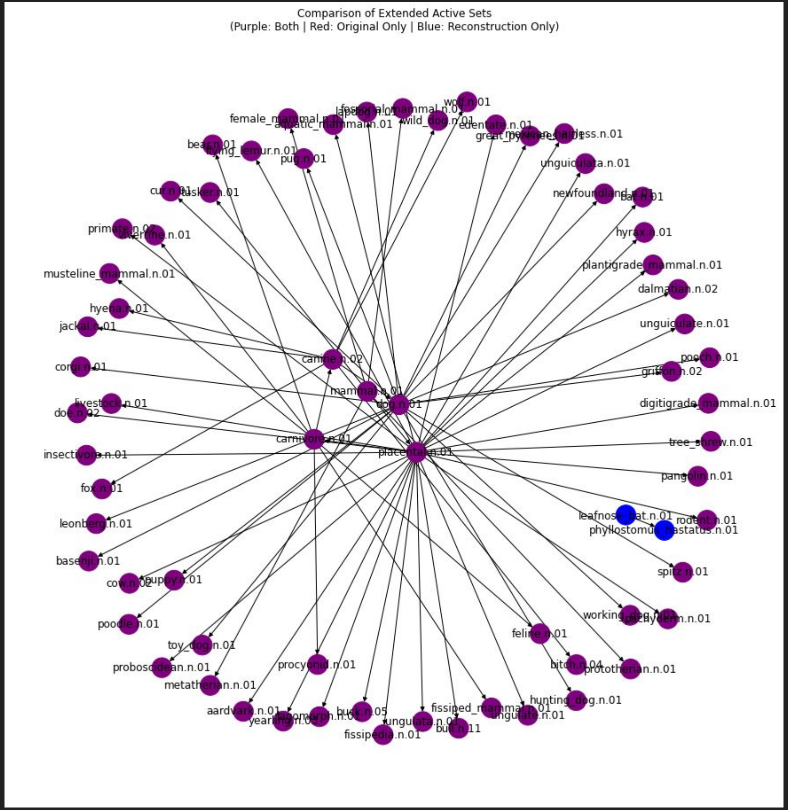
```
Chosen Sample Node:
pug.n.01

Original active synsets:
['canine.n.02', 'carnivore.n.01', 'dog.n.01', 'mammal.n.01', 'placental.n.0
1', 'pug.n.01']

Reconstructed active synsets:
['canine.n.02', 'carnivore.n.01', 'dog.n.01', 'mammal.n.01', 'phyllostomus_
hastatus.n.01', 'placental.n.01']
```

```
Reconstruction error (mean absolute difference): 0.0017
```

```
Precision=0.833, Recall=0.833, F1=0.833
```

Reconstruction Graphs (2 layers deep)





Results

Now reconstructing ‘dog.n.01’

Euclidean

```
Chosen Sample Node:
dog.n.01

Original active synsets:
['canine.n.02', 'carnivore.n.01', 'dog.n.01', 'mammal.n.01', 'placental.n.0
1']

Reconstructed active synsets:
['bovid.n.01', 'dog.n.01', 'mammal.n.01', 'odd-toed_ungulate.n.01', 'placen
tal.n.01', 'primate.n.02', 'rabbit-eared_bandicoot.n.01']
```

```
Reconstruction error (mean absolute difference): 0.0051
```

```
Precision=0.429, Recall=0.600, F1=0.500
```

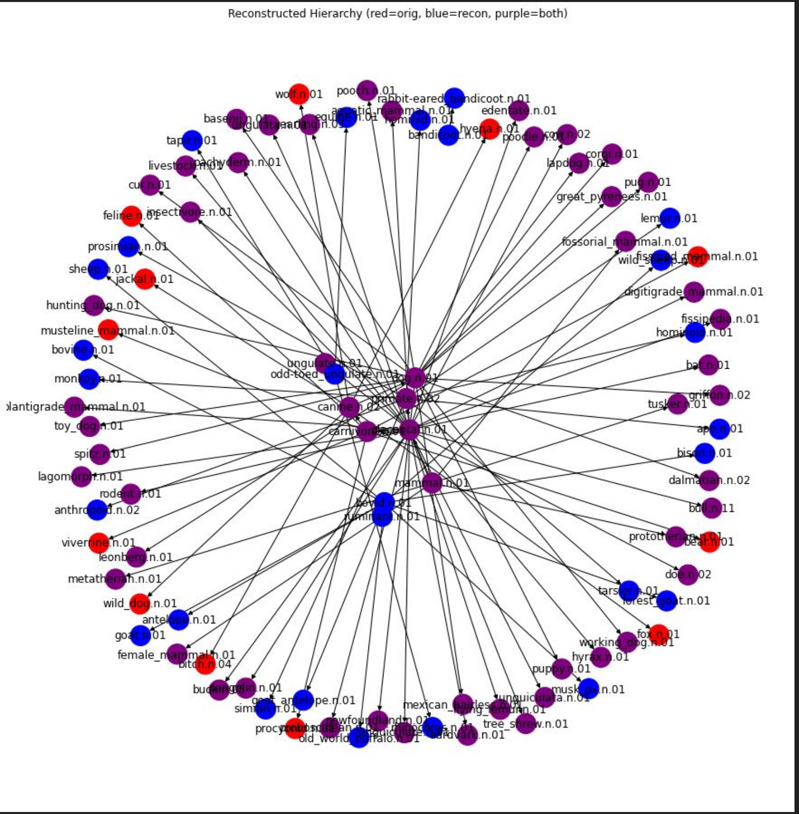
Hyperbolic

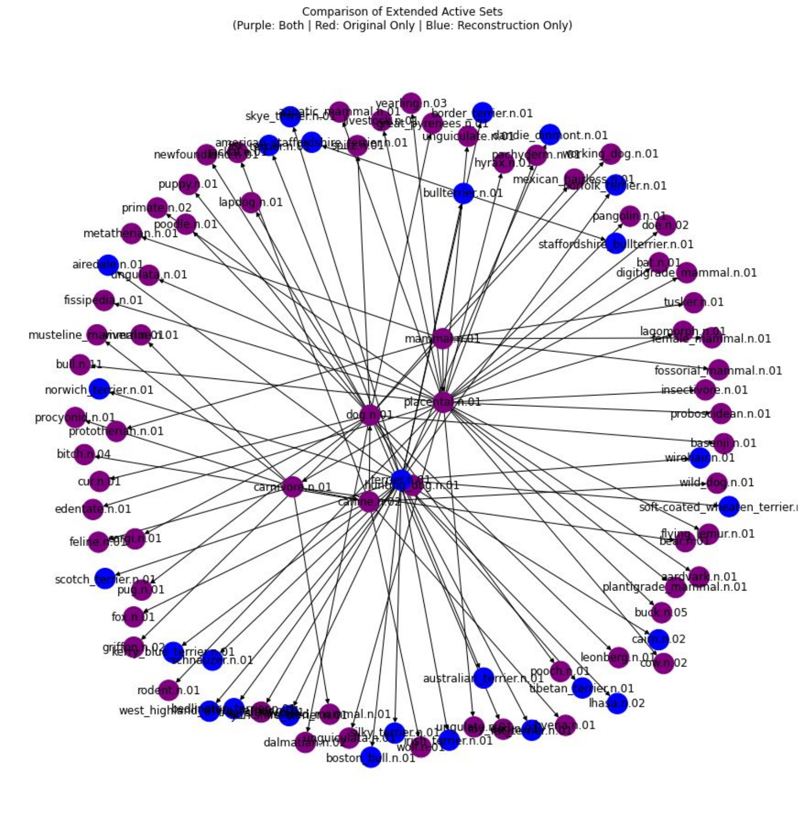
```
Chosen Sample Node:
dog.n.01

Original active synsets:
['canine.n.02', 'carnivore.n.01', 'dog.n.01', 'mammal.n.01', 'placental.n.0
1']

Reconstructed active synsets:
['canine.n.02', 'carnivore.n.01', 'dog.n.01', 'hunting_dog.n.01', 'mammal.
n.01', 'placental.n.01']
```

```
Reconstruction error (mean absolute difference): 0.0009
```

```
Precision=0.833, Recall=1.000, F1=0.909
```

Reconstruction Graphs (2 layers deep)





Challenges and Future Work

- Training Time
  - Hyperbolic arithmetic is more computationally intensive than standard float operations.
  - Future work: explore optimized implementations or approximations -- rewriting the model using PyTorch would enable GPU acceleration
- Future models could treat curvature as a hyperparameter or optimize it jointly with weights.
- A larger evaluation—e.g., across full WordNet, biomedical ontologies, or hierarchical image taxonomies—would provide stronger evidence of HRBM effectiveness.