Hyperbolic Restricted Boltzmann Machines for Hierarchical Learning

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CS 595: Computational Science Seminars

Agenda

1. Goals and motivation
2. Progress so far
3. Challenges Encountered
4. Next Steps

Research

Review literature on the use of hyperbolic numbers in machine learning

Prepare Data

Preprocess and embed data from wordnet noun hierarchy

Euclidean RBM

Design, implement, and test traditional euclidean RBM on wordnet data

Hyperbolic RBM

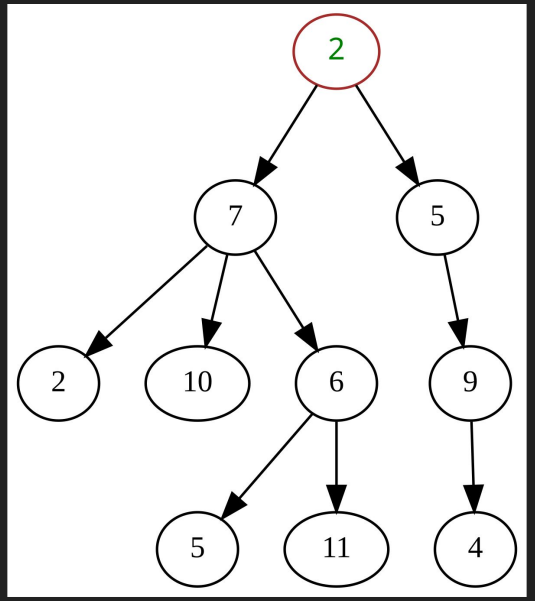
Implement Poincaré embeddings, sampling methods, hyperbolic energy function, etc. in code

Evaluation & Analysis

Compare euclidean and hyperbolic RBMs across metrics, analyze curvature, create visualizations

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.

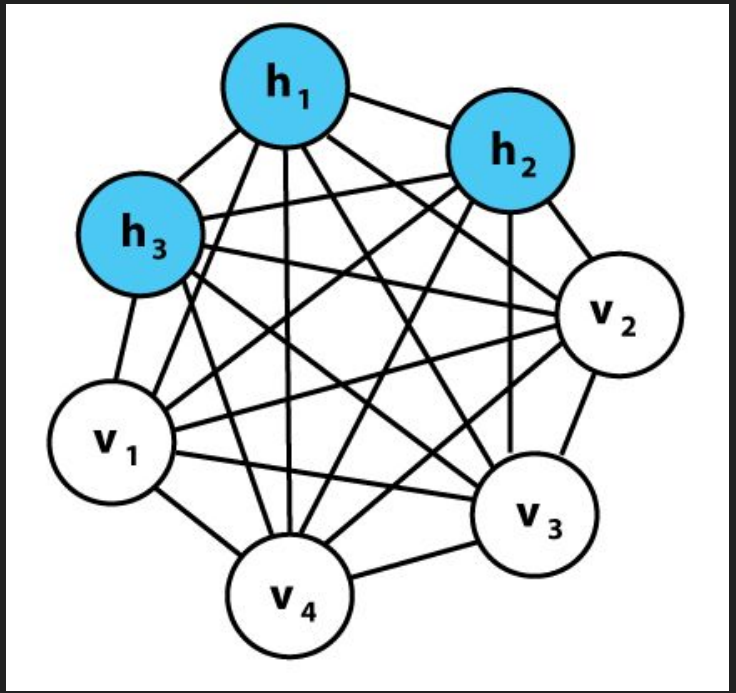


Literature Review

- 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.

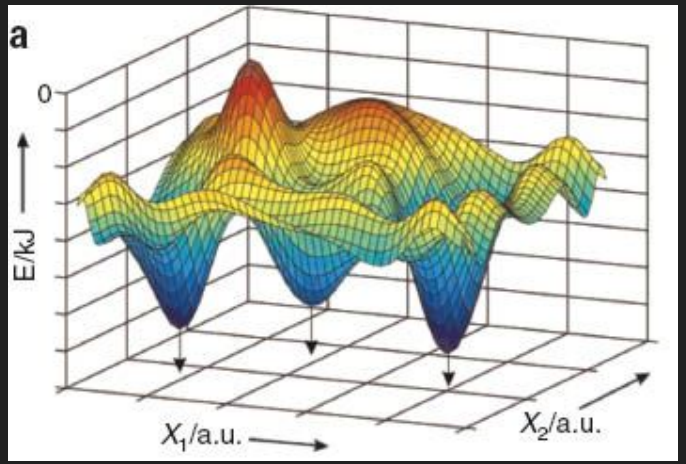


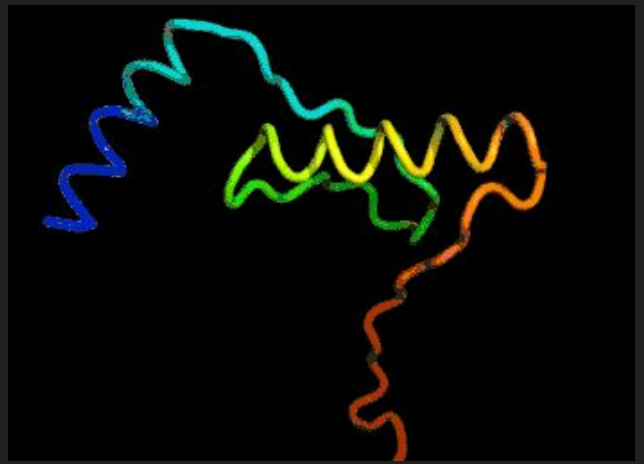
Energy Computation

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

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

Learning involves adjusting weights to reduce energy for training data



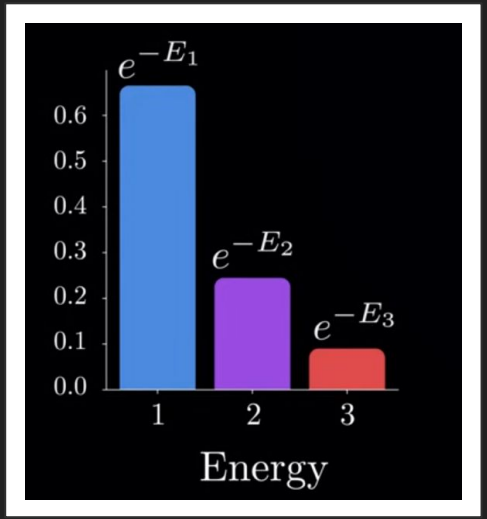


Energy Computation

- 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:

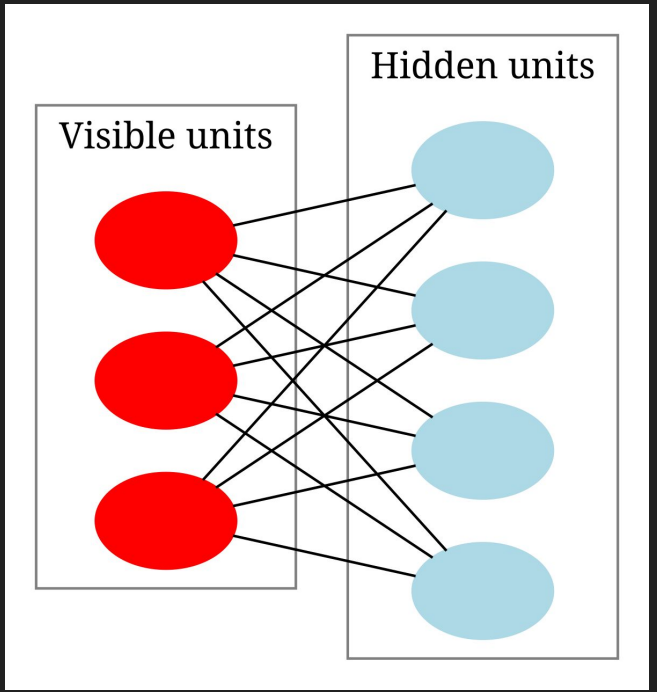
$$p(\mathbf{v}, \mathbf{h}) = \frac{\exp(-E(\mathbf{v}, \mathbf{h}))}{Z}$$

(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:

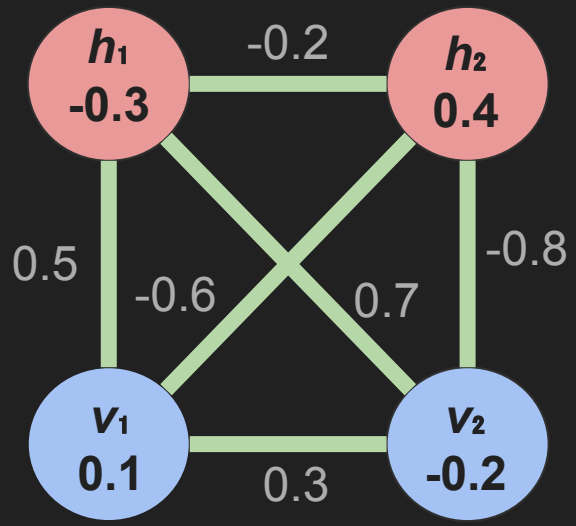
- x_1 = [1, 0] (Person 1 likes Movie A and dislikes Movie B)
- x_2 = [0, 1] (Person 2 dislikes Movie A and likes Movie B)
- x_3 = [1, 1] (Person 3 likes Movie A and Movie B)

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

We create the architecture to represent this data:

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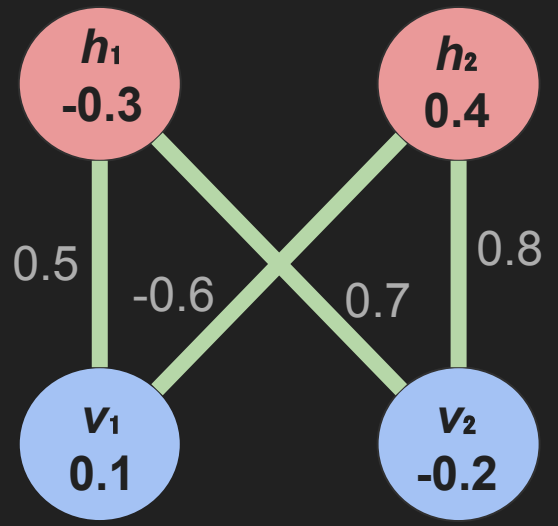
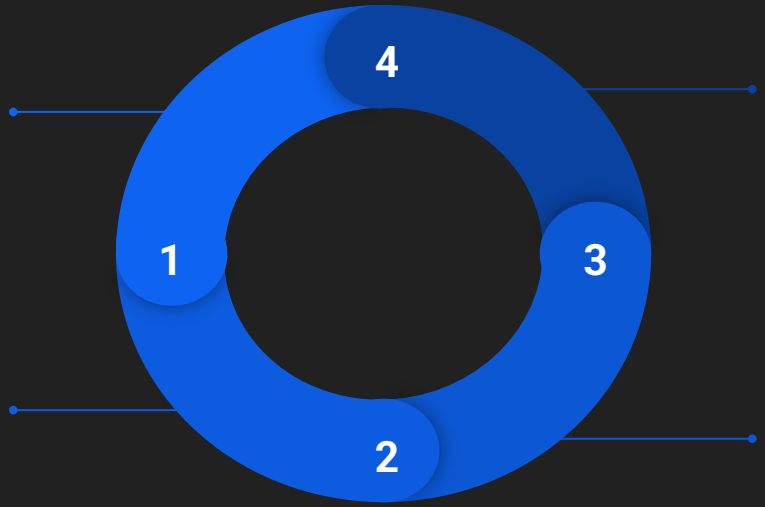


Initial values are chosen randomly or from domain knowledge

Training RBMs: Steps

0. Initialize weights and biases

1. Forward Pass
(Visible → Hidden)



4. Update weights
and biases

2. Reconstruct Input
(Hidden → Visible)

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:

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

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

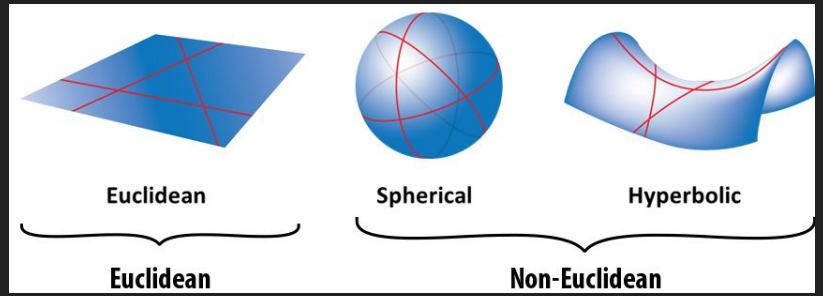
Legacy in Modern Machine Learning

- 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

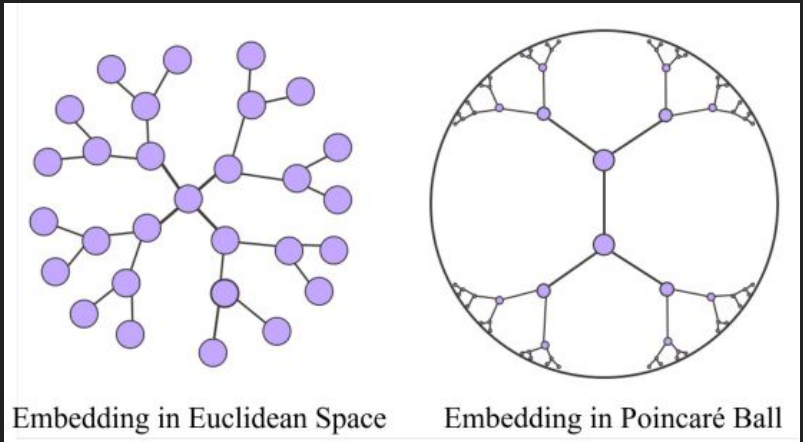
A Primer on Hyperbolic Geometry

- 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.



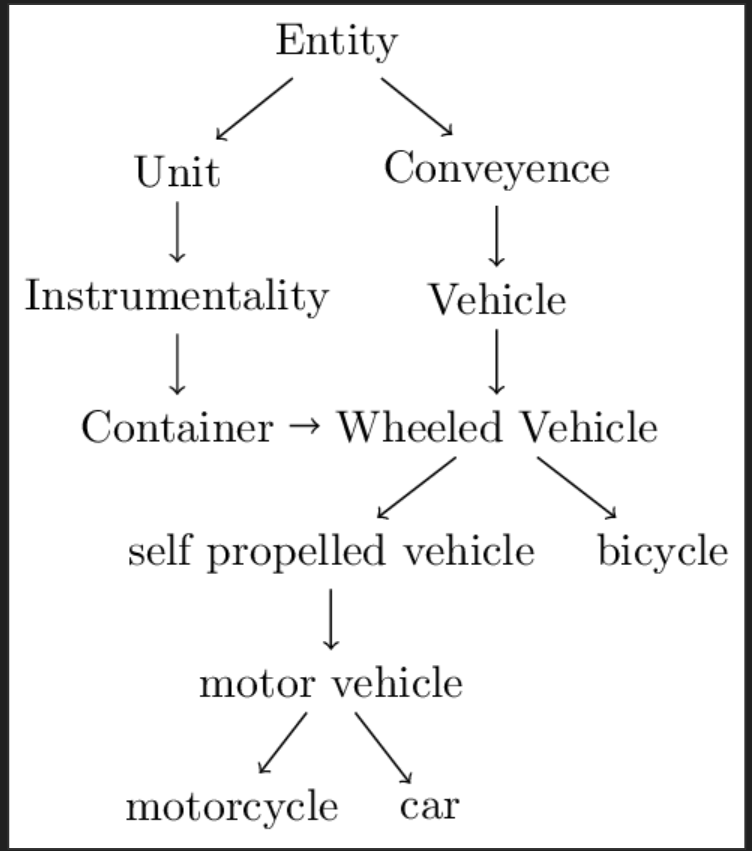
Hyperbolic Models: A Tool for Hierarchical Data

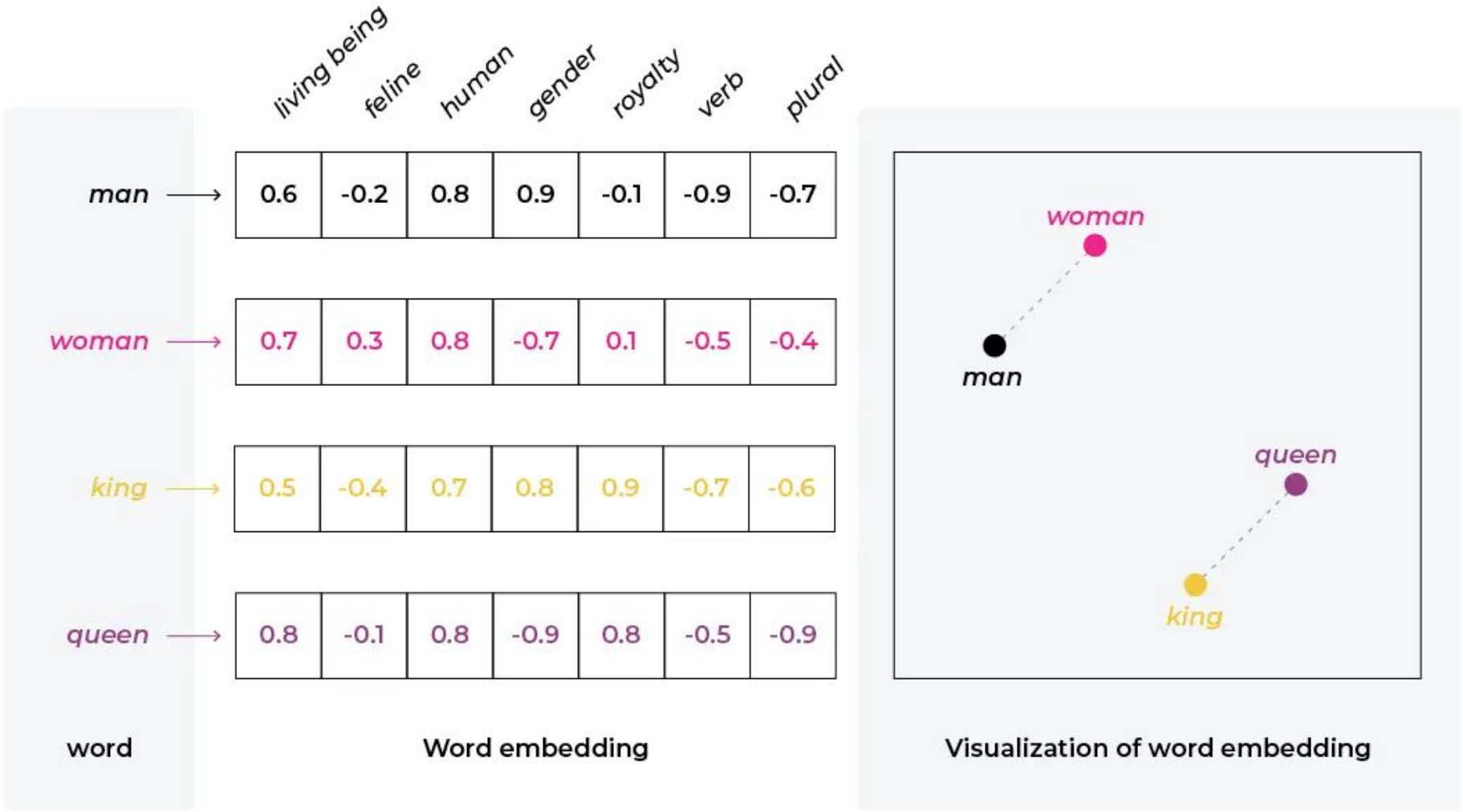
- Represent data points in hyperbolic space (e.g., Poincaré ball)
- Distance between points: $$d(x, y) = \operatorname{arcosh}\left(1 + 2\frac{\|x-y\|^2}{(1-\|x\|^2)(1-\|y\|^2)}\right)$$
- Efficient representation of hierarchies (fewer dimensions, lower distortion).

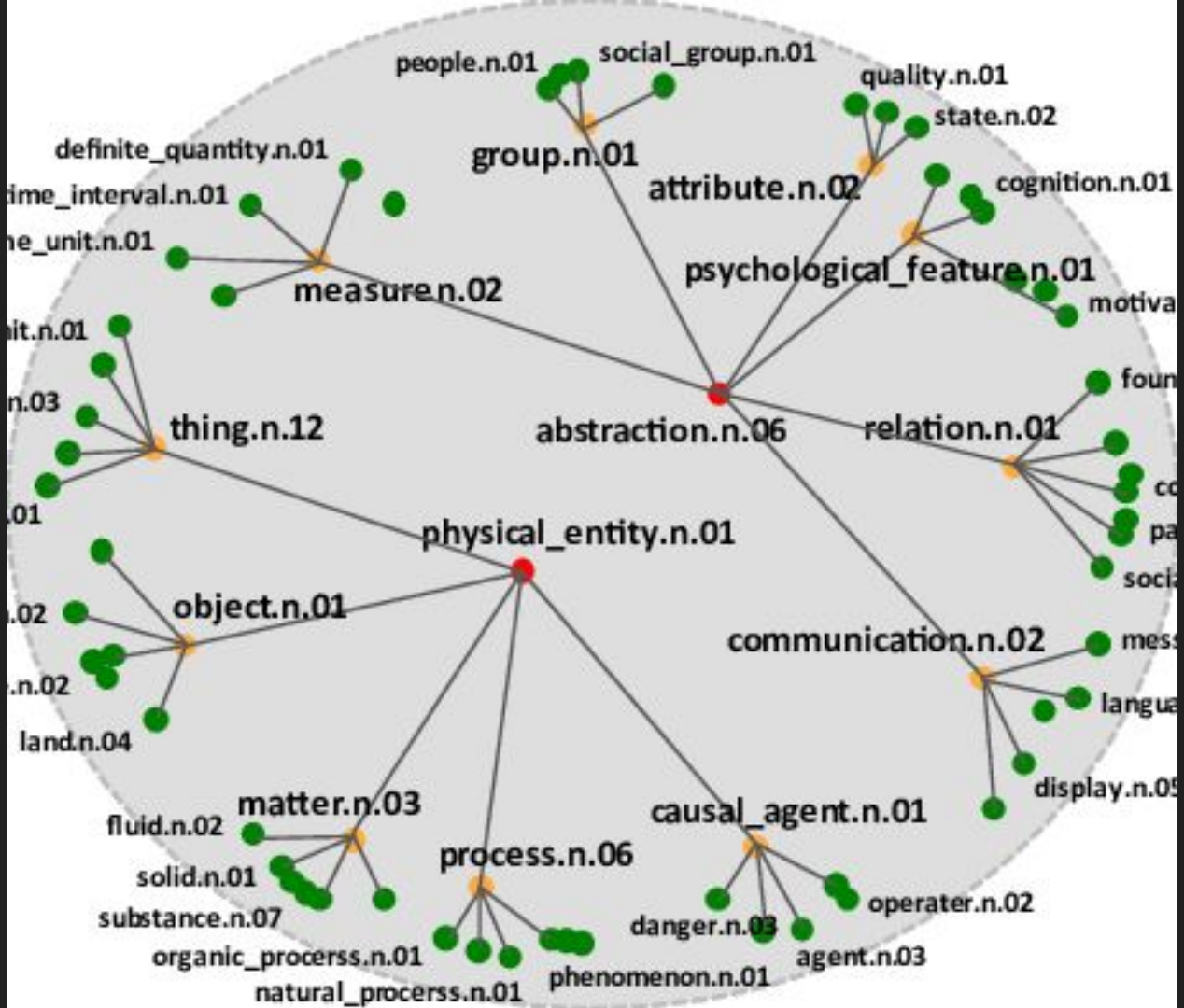


WordNet Hierarchy

- 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




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
woman
man
queen
king
Visualization of word embedding


people.n.01
social_group.n.01
quality.n.01
state.n.02
definite_quantity.n.01
group.n.01
attribute.n.02
cognition.n.01
measure.n.02
psychological_feature.n.01
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abstraction.n.06
relation.n.01
physical_entity.n.01
object.n.01
communication.n.02
land.n.04
matter.n.03
causal_agent.n.01
fluid.n.02
process.n.06
solid.n.01
substance.n.07
operater.n.02
danger.n.03
agent.n.03
organic_procerss.n.01
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.
- $\otimes$: Möbius addition (hyperbolic analog of vector addition).
- β: Scaling factor for curvature.

Model Design: Sampling Methods

Euclidean RBM:

- Gibbs Sampling: Sample $h \mid v$ and $v \mid h$ 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

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

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

- $\oplus$: Möbius addition.
- $\text{logit}_{\mathbb{H}}$: 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:

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

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

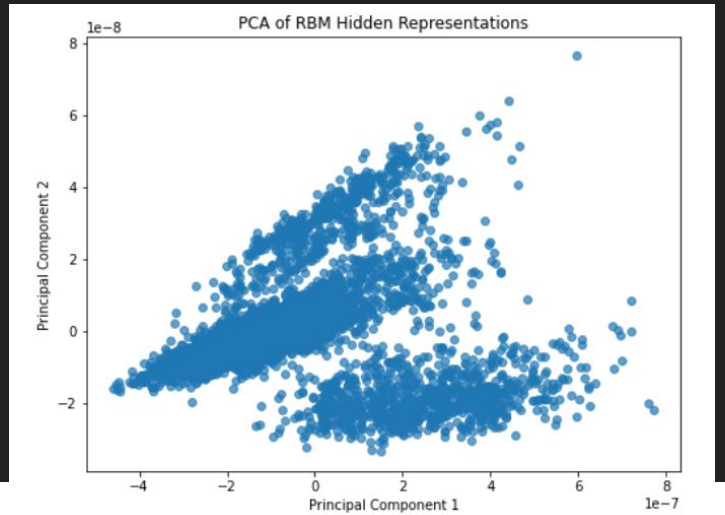
- Key Properties:
  - Gradients must respect the hyperbolic geometry (e.g., Riemannian optimization).
  - Optimization is more challenging due to curvature and numerical instability.

Implementation

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

Results

Using ‘animal.n.01’ as the root (3,999 synsets) in Euclidean RBM:




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

Original active synsets:
['animal.n.01', 'canine.n.02', 'carnivore.n.01', 'chordate.n.01', 'dog.n.01', 'domestic_animal.n.01', 'mammal.n.01', 'placen
tal.n.01', 'pug.n.01', 'vertebrate.n.01']

Reconstructed active synsets:
['animal.n.01', 'chordate.n.01', 'diapsid.n.01', 'mammal.n.01']
```

```
# Calculate a simple reconstruction error metric.
reconstruction_error = np.mean(np.abs(original_sample - reconstructed_sample))
print(f"\nReconstruction error (mean absolute difference): {reconstruction_error:.4f}")
```

```
Reconstruction error (mean absolute difference): 0.0020
```

Results

Using ‘dog.n.01’ as the root (190 synsets, ~15 min):

Euclidean RBM

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

Original active synsets:
['dog.n.01', 'pug.n.01']

Reconstructed active synsets:
['dog.n.01', 'hunting_dog.n.01', 'shepherd_dog.n.01', 'spaniel.n.01', 'terrier.n.01']
```

```
Reconstruction error (mean absolute difference): 0.0263
```

Hyperbolic RBM

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

Original active synsets:
['dog.n.01', 'pug.n.01']

Reconstructed active synsets:
['dog.n.01', 'springer_spaniel.n.01']
```

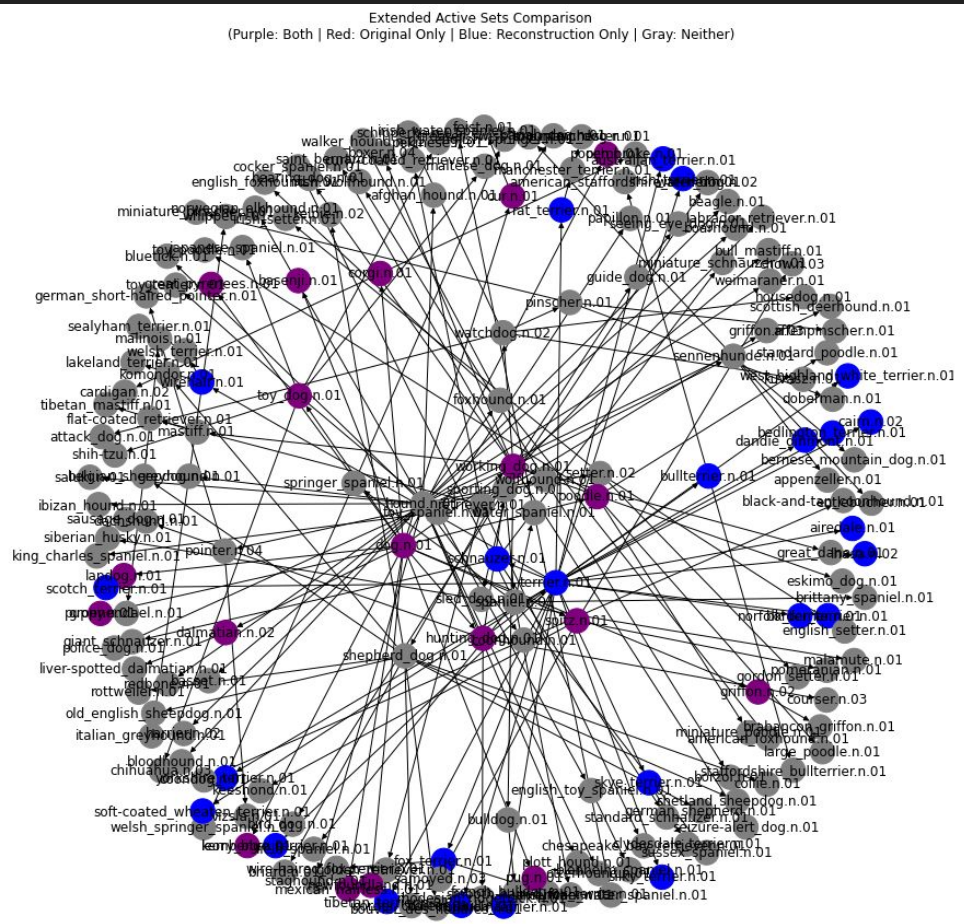
```
Reconstruction error (mean absolute difference): 0.0105
```

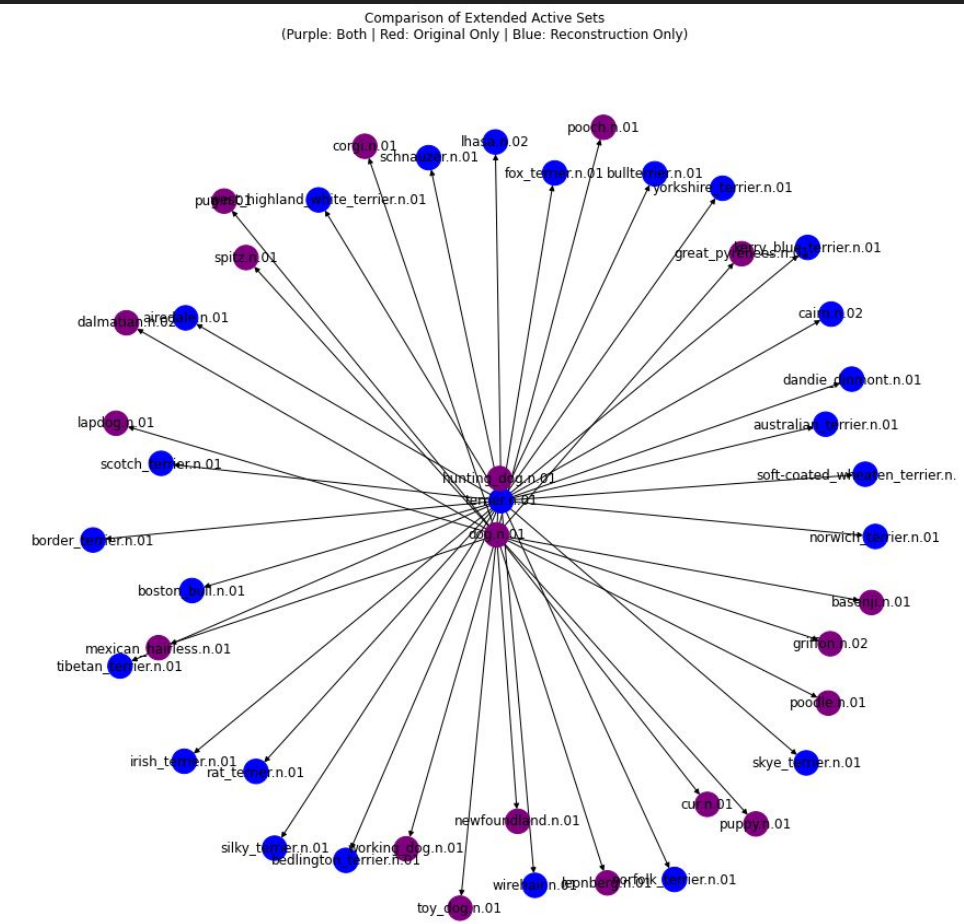
Results

Not many direct connections to ‘pug’, what if we compared 2 layers deep?

```
Extended original active synsets (direct + one extra layer):
['poodle.n.01', 'basenji.n.01', 'great_pyrenees.n.01', 'leonberg.n.01', 'mexican_hairless.n.01', 'lapdog.n.01', 'spitz.n.0
1', 'puppy.n.01', 'hunting_dog.n.01', 'toy_dog.n.01', 'pooch.n.01', 'corgi.n.01', 'cur.n.01', 'newfoundland.n.01', 'working_
dog.n.01', 'pug.n.01', 'dog.n.01', 'griffon.n.02', 'dalmatian.n.02']

Extended reconstructed active synsets (direct + one extra layer):
['spaniel.n.01', 'poodle.n.01', 'basenji.n.01', 'great_pyrenees.n.01', 'welsh_springer_spaniel.n.01', 'leonberg.n.01', 'mexi
can_hairless.n.01', 'lapdog.n.01', 'spitz.n.01', 'puppy.n.01', 'hunting_dog.n.01', 'toy_dog.n.01', 'pooch.n.01', 'corgi.n.0
1', 'cur.n.01', 'newfoundland.n.01', 'working_dog.n.01', 'pug.n.01', 'springer_spaniel.n.01', 'dog.n.01', 'english_springer.
n.01', 'griffon.n.02', 'dalmatian.n.02']
```


Extended Active Sets Comparison
(Purple: Both | Red: Original Only | Blue: Reconstruction Only | Gray: Neither)


Comparison of Extended Active Sets
(Purple: Both | Red: Original Only | Blue: Reconstruction Only)
hunting_dog.n.01
terrier.n.01
dog.n.01
corgi.n.01
schnauzer.n.01
lhasa.n.02
pooch.n.01
fox_terrier.n.01
bullterrier.n.01
yorkshire_terrier.n.01
great_pyrenees.n.01
cairn.n.02
dandie_dinmont.n.01
australian_terrier.n.01
soft-coated_wheaten_terrier.n.
norwich_terrier.n.01
basenji.n.01
griffon.n.02
poodle.n.01
skye_terrier.n.01
cur.n.01
puppy.n.01
norfolk_terrier.n.01
wirehair_pointing_griffon.n.01
toy_dog.n.01
newfoundland.n.01
silky_terrier.n.01
bedlington_terrier.n.01
irish_terrier.n.01
rat_terrier.n.01
mexican_hairless.n.01
tibetan_terrier.n.01
boston_bull.n.01
border_terrier.n.01
scotch_terrier.n.01
lapdog.n.01
dalmatian.n.02
airedale.n.01
spitz.n.01
pureblood.n.01
highland_white_terrier.n.01

Results

Now, I tried to run the models on the 1.2k synset “mammal” tree, but with only 2 epochs for the hyperbolic model. (~50 min)

Euclidean

```
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
```

Hyperbolic

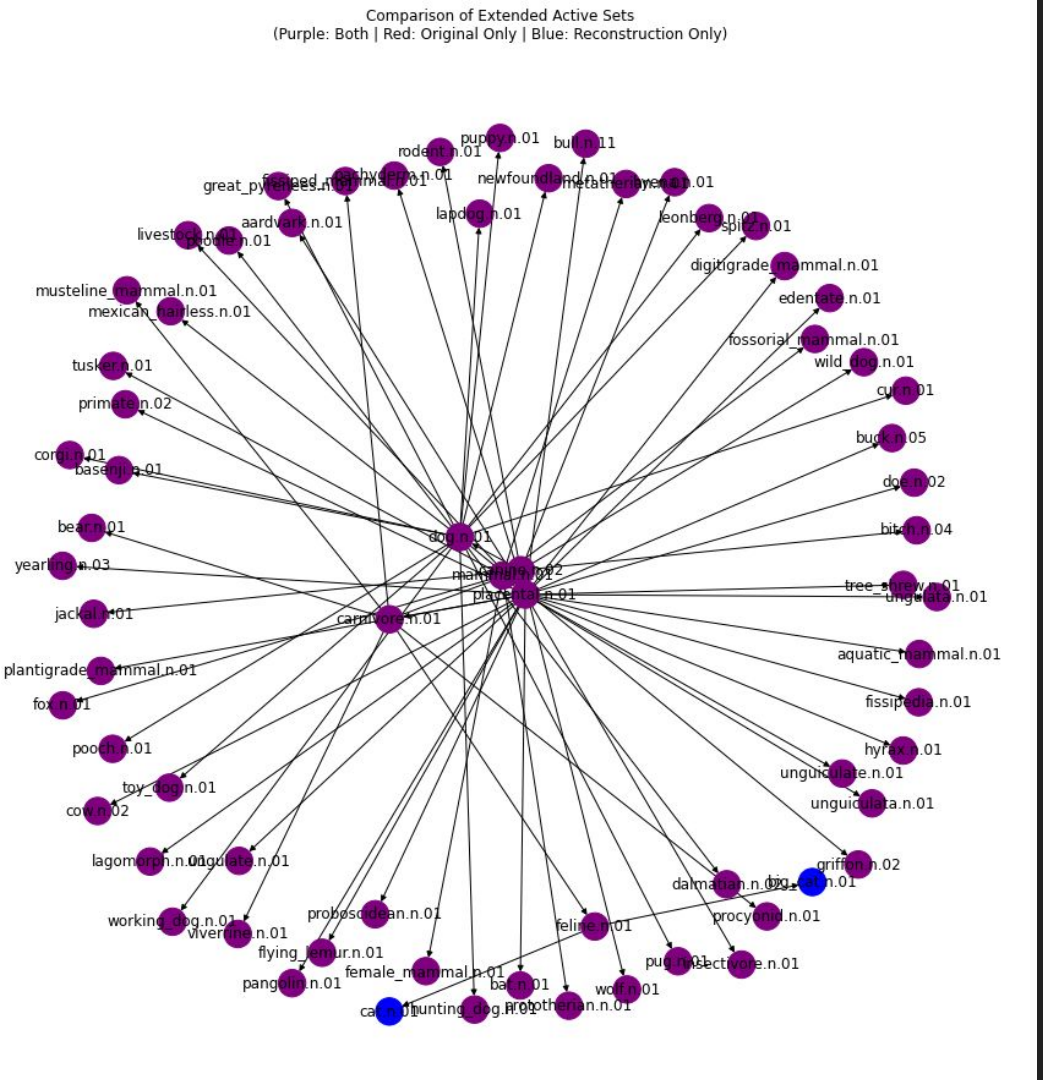
```
Chosen Sample Node:
pug.n.01

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', 'feline.n.01', 'mammal.n.01',
'placental.n.01']
```

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

Results


Comparison of Extended Active Sets
(Purple: Both | Red: Original Only | Blue: Reconstruction Only)
puppy.n.01
bull.n.11
rodent.n.01
great_pyrenees.n.01
newfoundland.n.01
metatherian.n.01
aardvark.n.01
landdog.n.01
leonberg.n.01
spitz.n.01
livestock.n.01
digitigrade_mammal.n.01
edentate.n.01
musteline_mammal.n.01
mexican_hairless.n.01
fossorial_mammal.n.01
wild_dog.n.01
tusker.n.01
cur.n.01
primate.n.02
buck.n.05
corgi.n.01
basenji.n.01
doe.n.02
bear.n.01
dog.n.01
bitch.n.04
yearling.n.03
tree_squirrel.n.01
placental.n.01
ungulata.n.01
jackal.n.01
carnivore.n.01
aquatic_mammal.n.01
plantigrade_mammal.n.01
fissipedia.n.01
fox.n.01
pooch.n.01
hyrax.n.01
unguiculate.n.01
toy_dog.n.01
unguiculata.n.01
cow.n.02
griffon.n.02
lagomorph.n.01
ungulate.n.01
dalmatian.n.02
big_dog.n.01
working_dog.n.01
proboscidean.n.01
procyonid.n.01
viverrine.n.01
feline.n.01
flying_lemur.n.01
pug.n.01
insectivore.n.01
female_mammal.n.01
pangolin.n.01
bat.n.01
wolf.n.01
hunting_dog.n.01
prototherian.n.01

Challenges and Future Work

- Hyperbolic Activation Function
  - Currently uses a standard sigmoid on the real part.
  - A fully hyperbolic activation (affecting both components) may boost performance but adds complexity.
- Training Time
  - Hyperbolic arithmetic is more computationally intensive than standard float operations.
  - Future work: explore optimized implementations or approximations.
- Reconstruction Quality
  - Plan to benchmark HRBM vs. Bernoulli RBM on reconstruction quality, fidelity, and robustness.
  - Future Work: research and/or develop reconstruction metrics
- Future Work: test difference levels of curvature in hyperbolic RBM