

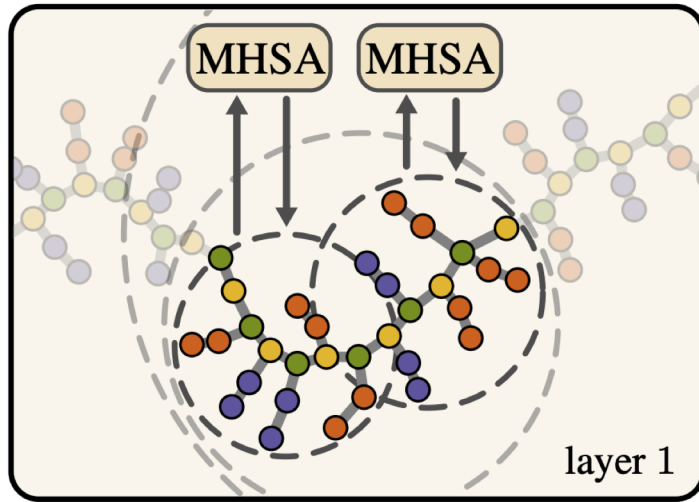


# Designing Hierarchies for Optimal Hyperbolic Embedding

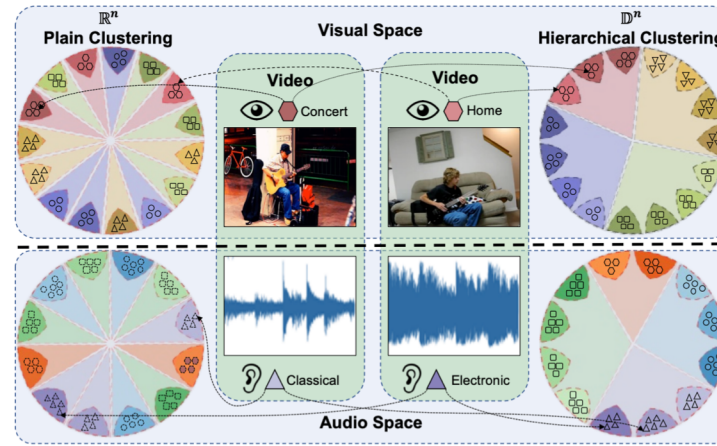
**Melika Ayoughi**, Max van Spengler, Pascal Mettes, and Paul Groth  
m.ayoughi@uva.nl

June 3<sup>rd</sup> 2025

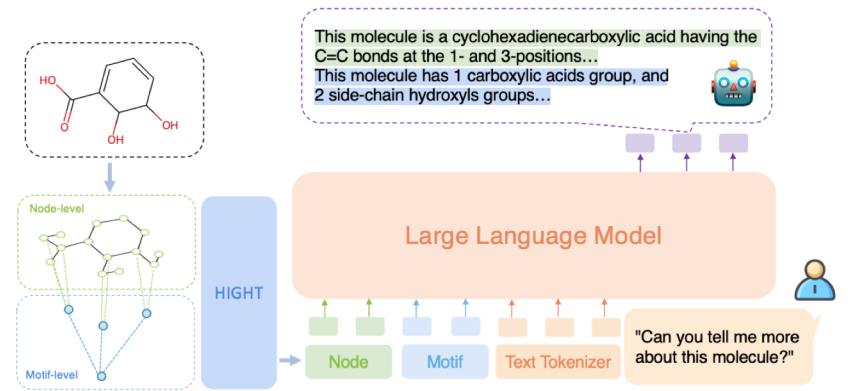
# Embedded Hierarchies



[Zhdanov et al. ICML 2025]



[Teng et al. ICCV 2023]

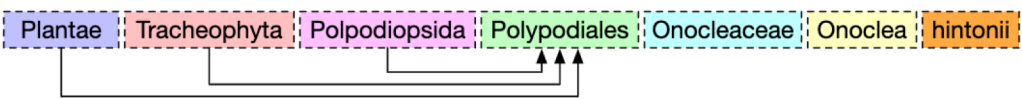


[Chen et al. ICML 2025]

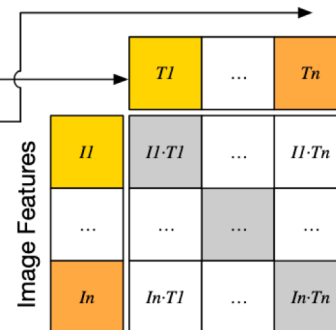
(a) Taxonomic Labels

| Kingdom | Phylum       | Class          | Order        | Family      | Genus   | Species    |
|---------|--------------|----------------|--------------|-------------|---------|------------|
| Plantae | Tracheophyta | Polypodiopsida | Polypodiales | Onocleaceae | Onoclea | sensibilis |
| Plantae | Tracheophyta | Polypodiopsida | Polypodiales | Onocleaceae | Onoclea | hintonii   |

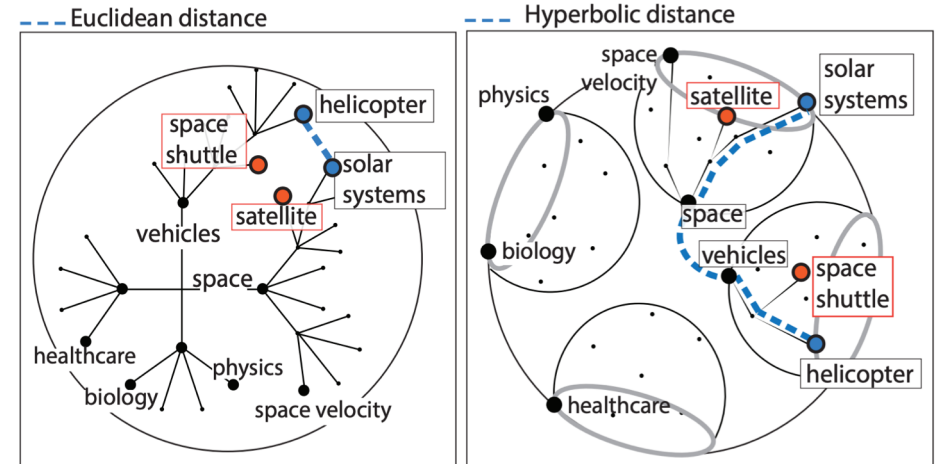
(b) Autoregressive Representations



(c) Contrastive Objective



[Stevens et al. CVPR 2024]

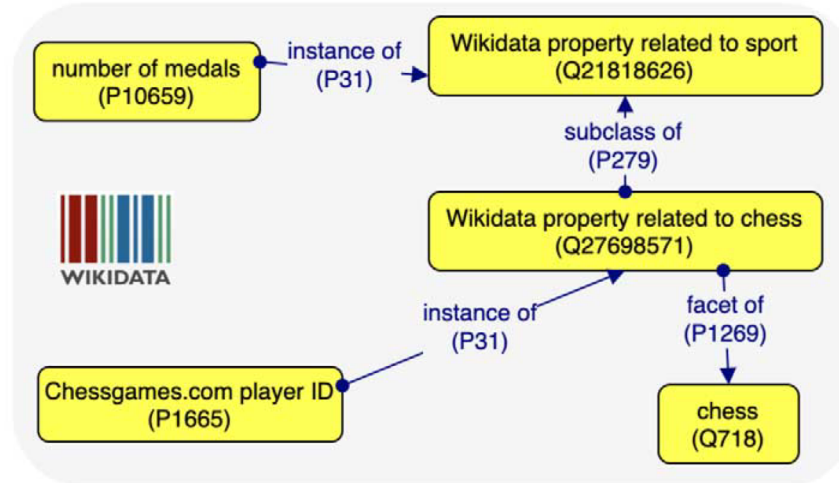


[Shahid et al. ACL 2023]

# Knowledge Graphs and Ontologies

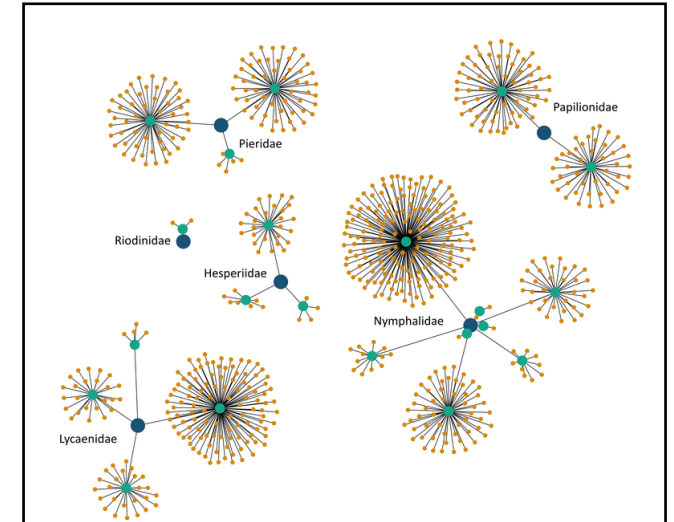


[[schema.org](https://schema.org)]



[Carriero et al. Semantic Web 2024]

**WordNet**  
A Lexical Database for English



[The ETHEC entomological hierarchy]

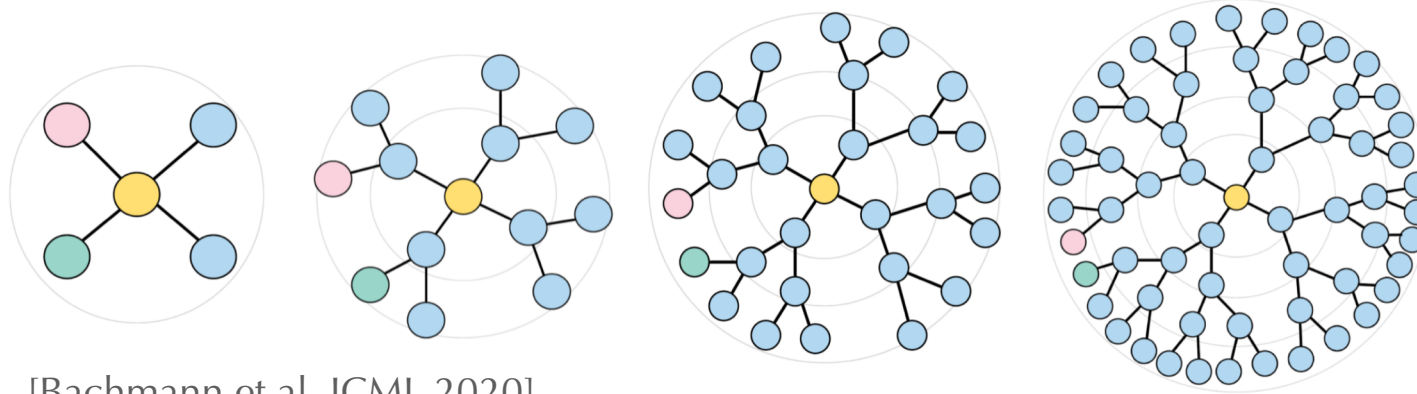
Most methods use the hierarchies **as is**, however, ontology engineers have **control** over the hierarchy.



How can hierarchies be designed to suite ML tasks?

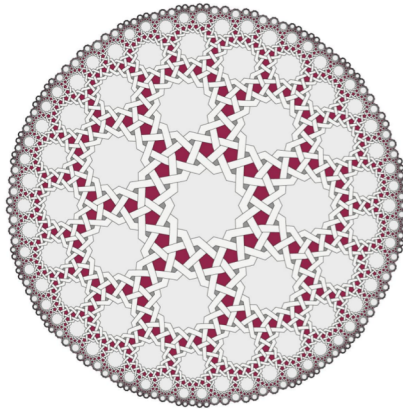
# Optimal geometry for hierarchical representation

Euclidean



[Bachmann et al. ICML 2020]

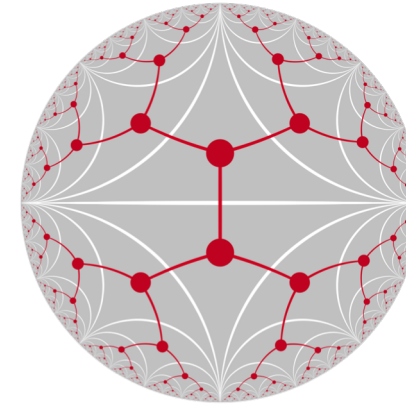
Hyperbolic



[KAPLAN et al. TOG 2004]



[M.C.Escher's "Circle Limit III"]



“Hyperbolic space can be thought of as a **continuous** analogue to **discrete trees**”



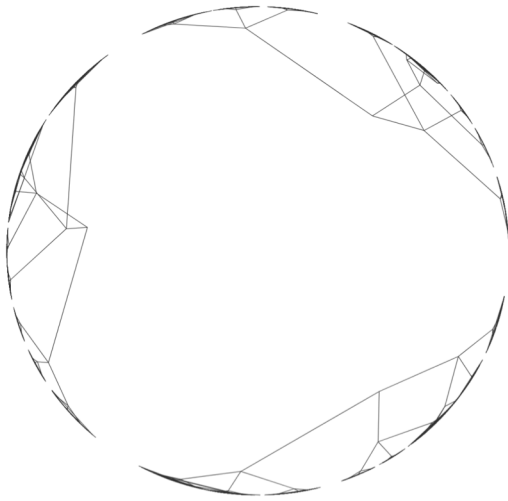
# Controlled Experiment Setup

Hyperbolic Embedding Methods, Hierarchies, Evaluation Metrics

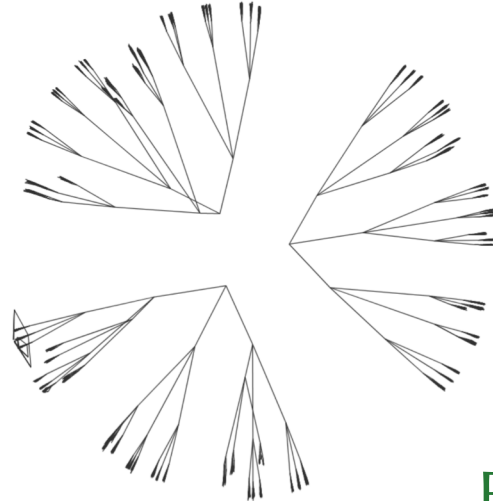
# Hyperbolic Embedding Methods

## Gradient-based

Poincaré



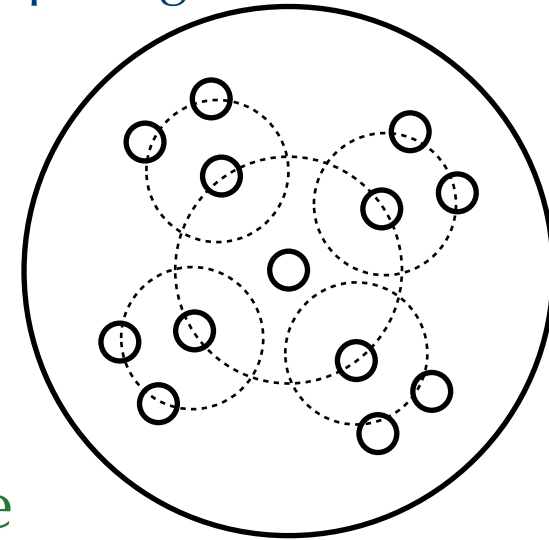
Entailment



## Construction-based

Precomputing

Hadamard



Enforce structure

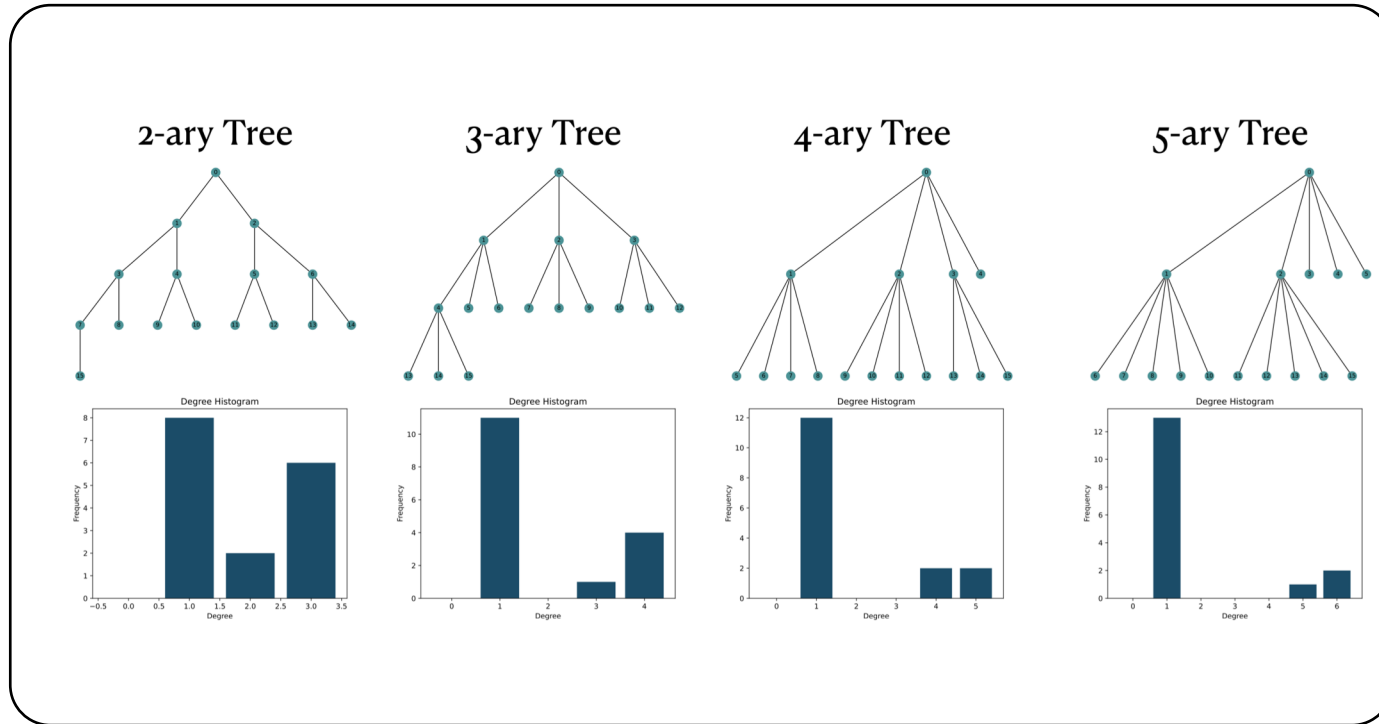
[Ganea et al. ICML 2018]

- + General-purpose
- Quality not guaranteed

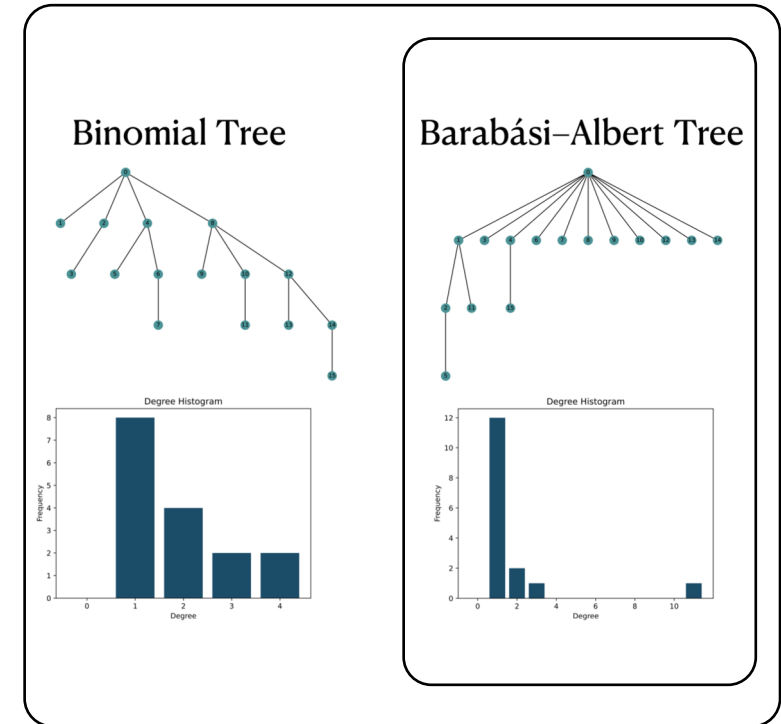
- + High-quality embeddings
- + Fast
- + Preserve original hierarchy structure
- Arbitrary-precision arithmetic

# Diverse Hierarchies

Long-tailed



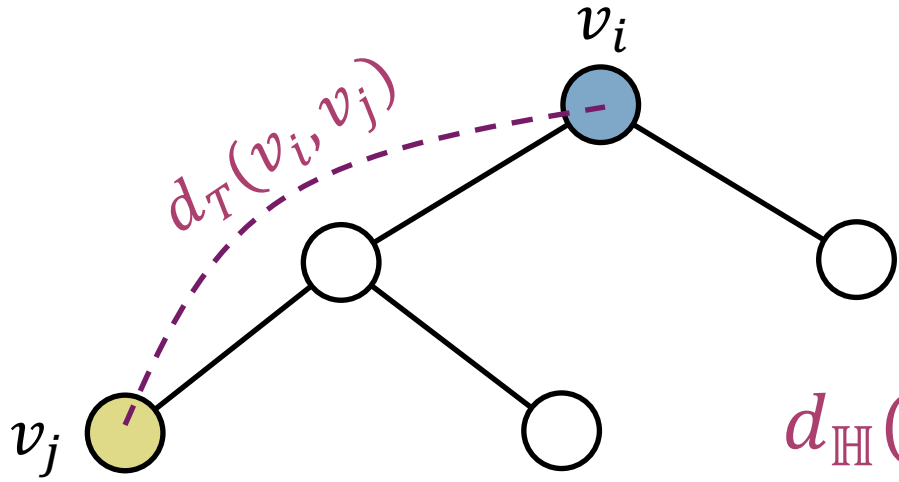
Balanced



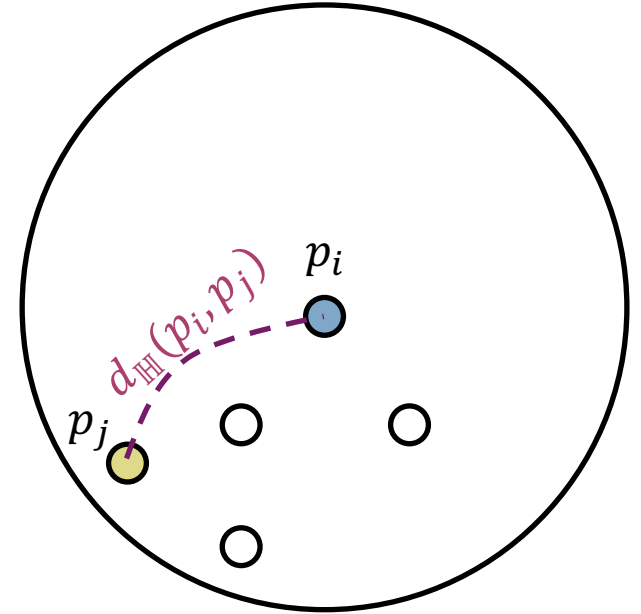
Imbalanced



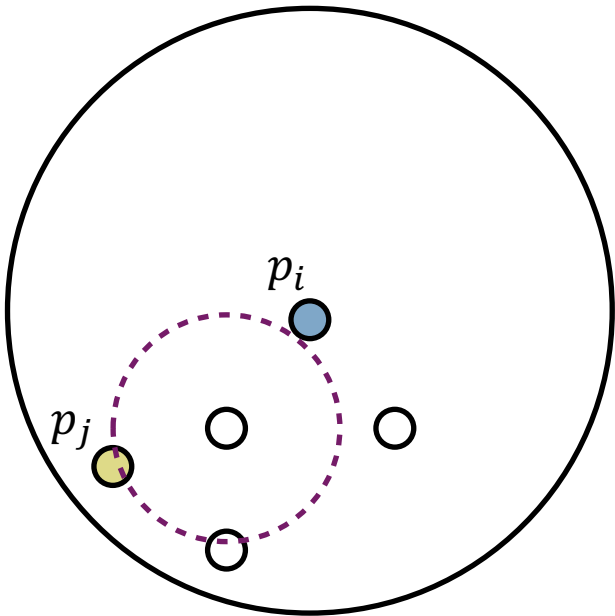
# Evaluation Metrics



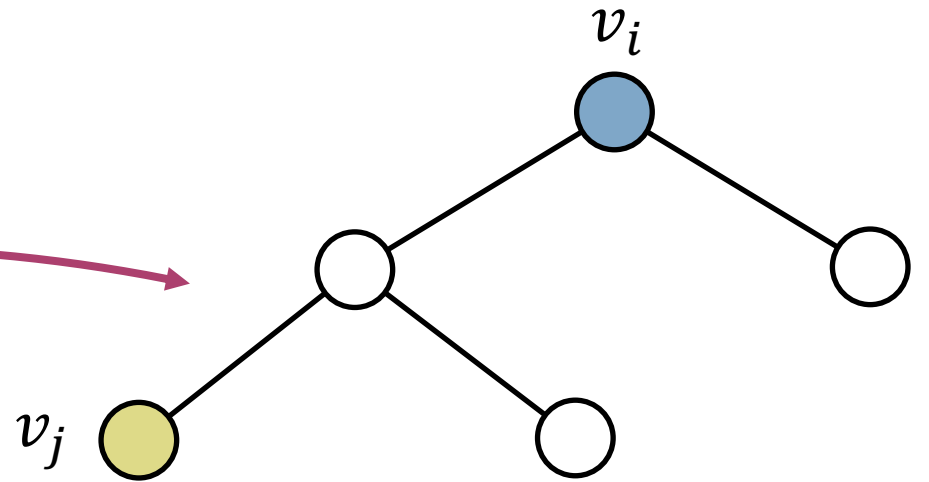
$$d_H(p_i, p_j) \propto d_T(v_i, v_j)$$



$\downarrow D_{avg} \downarrow D_{wc}$   
Distortion



Reconstruct  $\rightarrow$



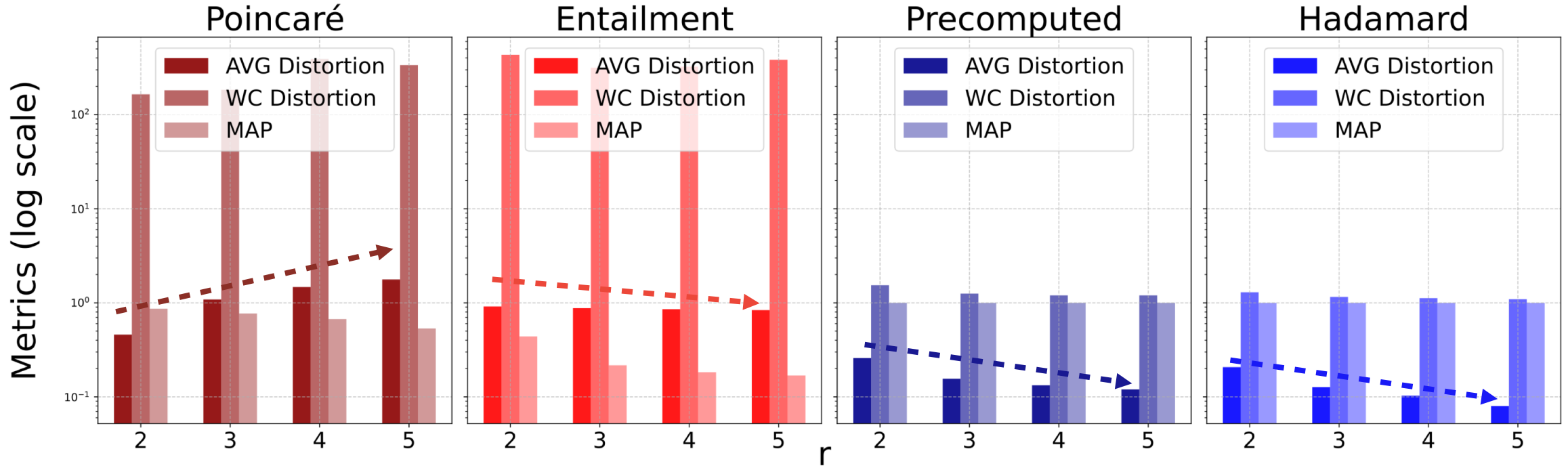
$\uparrow MAP$   
Reconstruction



# Experiments

# Depth or Width?

Cheatsheet:  
 $\downarrow D_{avg} \downarrow D_{wc} \uparrow MAP$



- I. All methods except for Poincaré: **wide and shallow** hierarchies have lower distortion.
- II. **Construction-based** methods paired with **wide** hierarchies achieve **optimal** embeddings.

# What is the impact of more nodes on embedding quality?

Cheatsheet:  
↓  $D_{avg}$  ↓  $D_{wc}$  ↑  $MAP$

|                   | Gradient-based |       |       |            |       |       | Construction-based |       |       |          |       |       |
|-------------------|----------------|-------|-------|------------|-------|-------|--------------------|-------|-------|----------|-------|-------|
|                   | Poincaré       |       |       | Entailment |       |       | Precomputed        |       |       | Hadamard |       |       |
|                   | 256            | 512   | 1024  | 256        | 512   | 1024  | 256                | 512   | 1024  | 256      | 512   | 1024  |
| <b>Balanced</b>   |                |       |       |            |       |       |                    |       |       |          |       |       |
| 2-ary             | 0.880          | 0.459 | 0.229 | 0.816      | 0.914 | 0.960 | 0.220              | 0.259 | 0.300 | 0.176    | 0.207 | 0.240 |
| 3-ary             | 1.439          | 1.085 | 0.752 | 0.742      | 0.878 | 0.940 | 0.124              | 0.156 | 0.160 | 0.102    | 0.127 | 0.130 |
| 4-ary             | 2.129          | 1.471 | 1.092 | 0.695      | 0.855 | 0.928 | 0.102              | 0.133 | 0.137 | 0.079    | 0.103 | 0.105 |
| 5-ary             | 2.472          | 1.770 | 1.385 | 0.657      | 0.837 | 0.919 | 0.115              | 0.120 | 0.156 | 0.078    | 0.080 | 0.103 |
| <b>Imbalanced</b> |                |       |       |            |       |       |                    |       |       |          |       |       |
| Binomial          | 1.736          | 1.439 | 0.988 | 0.717      | 0.863 | 0.932 | 0.207              | 0.249 | 0.298 | 0.161    | 0.186 | 0.211 |
| BA                | 3.444          | 2.791 | 2.206 | 0.595      | 0.802 | 0.903 | 0.108              | 0.140 | 0.178 | -        | -     | -     |

A strong **increase in semantic complexity** has **minimal impact** on embedding quality.

# Balanced or Imbalanced?

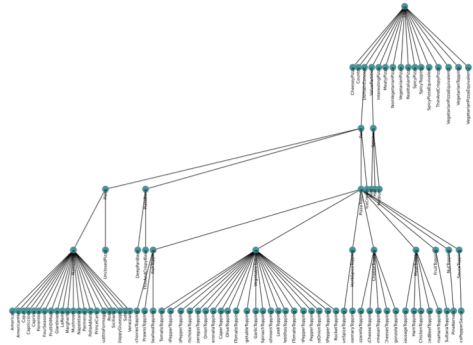
Cheatsheet:  
 $\downarrow D_{avg}$   $\downarrow D_{wc}$   $\uparrow MAP$   
 best and worst

|                   | Gradient-based |          |       |            |          |       | Construction-based |          |     |           |          |     |
|-------------------|----------------|----------|-------|------------|----------|-------|--------------------|----------|-----|-----------|----------|-----|
|                   | Poincaré       |          |       | Entailment |          |       | Precomputed        |          |     | Hadamard  |          |     |
|                   | $D_{avg}$      | $D_{wc}$ | MAP   | $D_{avg}$  | $D_{wc}$ | MAP   | $D_{avg}$          | $D_{wc}$ | MAP | $D_{avg}$ | $D_{wc}$ | MAP |
| <b>Balanced</b>   |                |          |       |            |          |       |                    |          |     |           |          |     |
| 2-ary             | 0.459          | 164.777  | 0.866 | 0.914      | 434.177  | 0.439 | 0.259              | 1.539    | 1   | 0.207     | 1.297    | 1   |
| 3-ary             | 1.085          | 183.974  | 0.770 | 0.878      | 316.338  | 0.217 | 0.156              | 1.252    | 1   | 0.127     | 1.155    | 1   |
| 4-ary             | 1.471          | 390.397  | 0.671 | 0.855      | 323.967  | 0.183 | 0.133              | 1.201    | 1   | 0.103     | 1.121    | 1   |
| 5-ary             | 1.770          | 336.711  | 0.534 | 0.837      | 383.626  | 0.169 | 0.120              | 1.201    | 1   | 0.080     | 1.092    | 1   |
| <b>Imbalanced</b> |                |          |       |            |          |       |                    |          |     |           |          |     |
| Binomial          | 1.439          | 69.530   | 0.171 | 0.863      | 224.731  | 0.304 | 0.249              | 1.542    | 1   | 0.186     | 1.257    | 1   |
| BA                | 2.791          | 3607.95  | 0.020 | 0.802      | 731.914  | 0.231 | 0.140              | 1.329    | 1   | -         | -        | -   |

Better to have a wide imbalanced tree than a deep balanced one!

# Case study: The Pizza and ImageNet ontologies

Pizza reorganized



ImageNet reorganized



Cheatsheet:  
 $\downarrow D_{avg}$   $\downarrow D_{wc}$   $\uparrow MAP$

|                      | Gradient-based |           |       |            |          |       | Construction-based |          |       |              |              |          |
|----------------------|----------------|-----------|-------|------------|----------|-------|--------------------|----------|-------|--------------|--------------|----------|
|                      | Poincaré       |           |       | Entailment |          |       | Precomputed        |          |       | Hadamard     |              |          |
|                      | $D_{avg}$      | $D_{wc}$  | MAP   | $D_{avg}$  | $D_{wc}$ | MAP   | $D_{avg}$          | $D_{wc}$ | MAP   | $D_{avg}$    | $D_{wc}$     | MAP      |
| <b>Pizza</b>         |                |           |       |            |          |       |                    |          |       |              |              |          |
| Original             | 3.321          | 7066.671  | 0.059 | -          | -        | -     | -                  | -        | -     | -            | -            | -        |
| + single inheritance | 3.387          | 10509.346 | 0.051 | 0.499      | 511.594  | 0.195 | 0.234              | 1.538    | 1     | 0.126        | 1.180        | 1        |
| + reorganized        | 3.422          | 9343.566  | 0.045 | 0.452      | 1454.972 | 0.164 | 0.167              | 1.329    | 1     | <b>0.089</b> | <b>1.118</b> | <b>1</b> |
| <b>ImageNet</b>      |                |           |       |            |          |       |                    |          |       |              |              |          |
| Original             | 0.809          | 3983.563  | 0.087 | -          | -        | -     | -                  | -        | -     | -            | -            | -        |
| + single inheritance | 0.722          | 2745.952  | 0.220 | 0.961      | 2364.827 | 0.293 | 0.725              | 885.622  | 0.725 | 0.297        | 1.647        | 1        |
| + reorganized        | 1.008          | 12715.625 | 0.156 | 0.955      | 4096.000 | 0.164 | 0.507              | 2.698    | 1     | <b>0.171</b> | <b>1.232</b> | <b>1</b> |

- I. Poincaré: only method to handle multiple inheritance
- II. Hierarchy reorganization leads to better distortion and MAP



# Recommendations

- ✓ Design hierarchies for width
- ✓ Do not worry about balance
- ✓ Hyperbolic embeddings can handle additional node complexity
- ✓ Avoid multiple inheritance; o/w limited to Poincaré method



# Wrapping up my PhD - Looking for What's Next!



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[m.ayoughi@uva.nl](mailto:m.ayoughi@uva.nl)

