Using hyperbolic large-margin classifiers for biological link prediction

SemDeep-5 @ IJCAI 2019

Asan Agibetov, Georg Dorffner, Matthias Samwald

Institute für Artificial Intelligence and Decision Support - Medical University of Vienna, Austria

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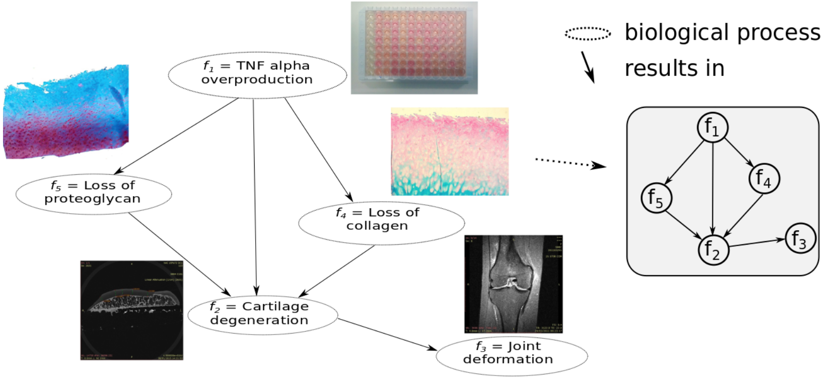
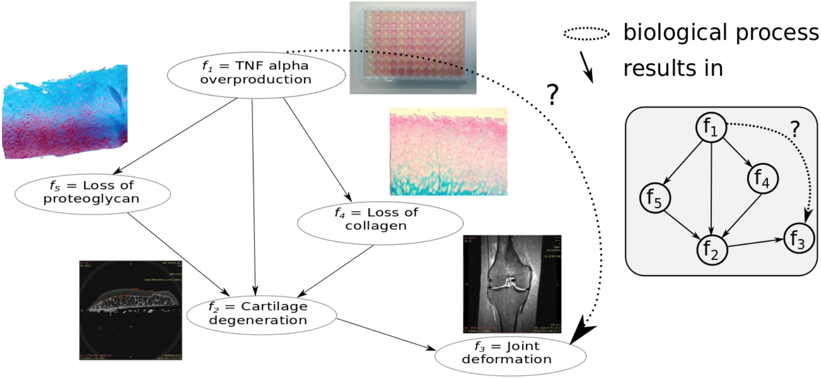
Representing biological knowledge[1]

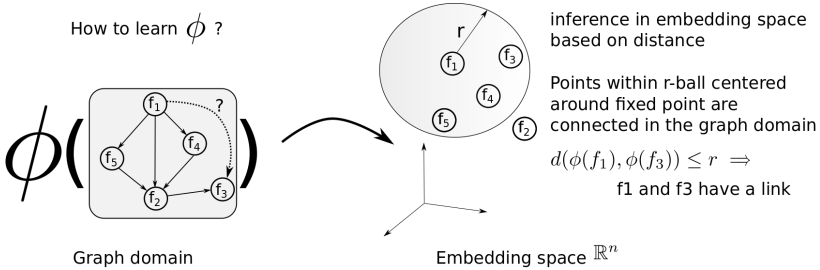


[1]"Shared hypothesis testing", Agibetov et al., J. Biomed. Sem., 2018

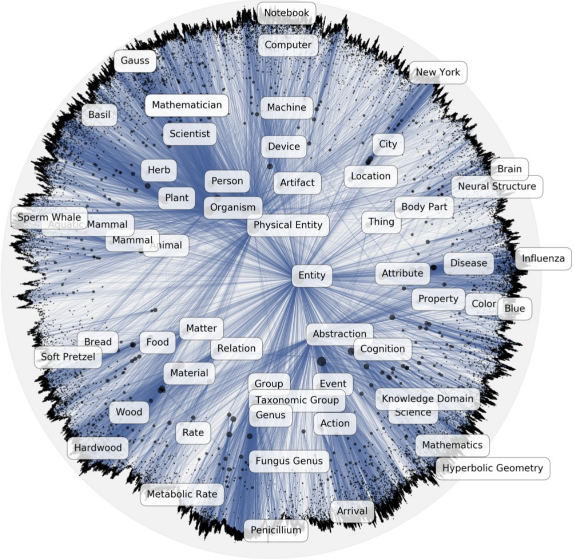
Biological link prediction



Link prediction as distance based inference in embedding space

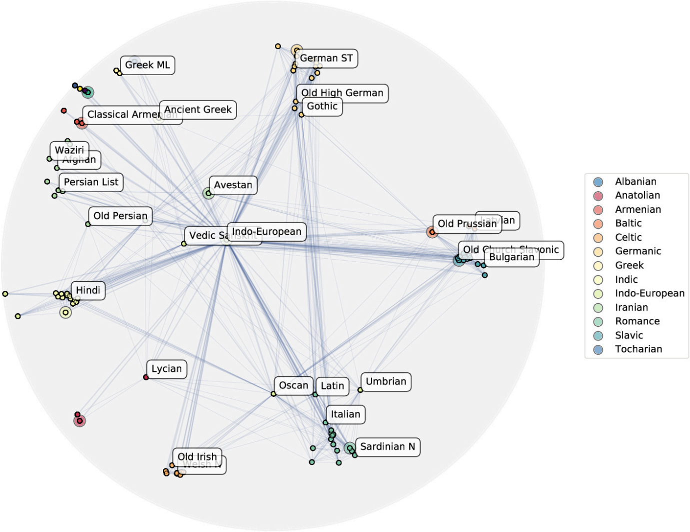


Representation learning in Hyperbolic space



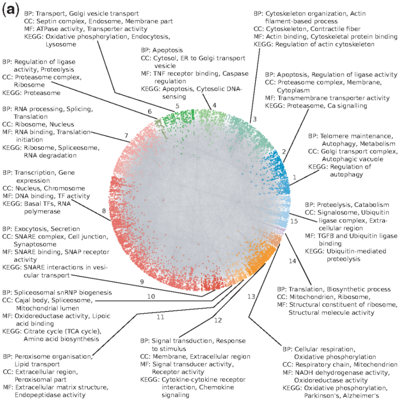
Nickel and Kiela. NIPS 2017

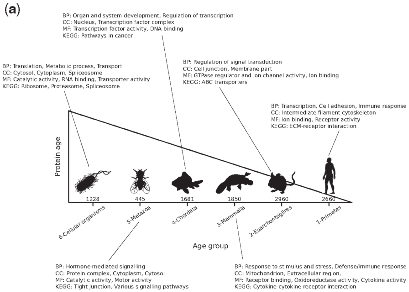
Hierarchical relationship from hyperbolic embeddings



Nickel and Kiela. ICML 2018

Clusters of proteins and age groups from hyperbolic coordinates





Lobato et al. Bioinformatics 2018

Hyperbolic embeddings

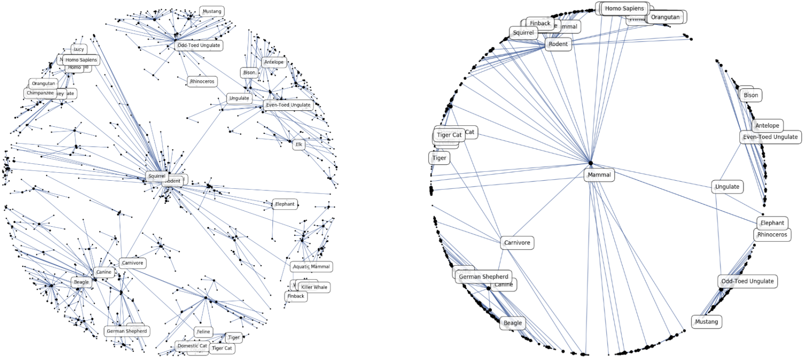
Same as in Euclidean case we try to learn a *link estimator* $Q(u, v) \mapsto [0, 1]$ (u, v node pairs) with MLE

- $Pr(G) = \prod_{(u,v) \in E_{train}} Q(u, v) \prod_{(u,v) \notin E_{train}} 1 - Q(u, v)$
- If Q perfect estimator then $Pr(x) = 1$ iff $x = G$ (i.e., graph can be fully reconstructed)

Embeddings are parameters Θ of link estimator Q; trained with cross-entropy loss $\mathcal{L}$ and negative sampling

- $\mathcal{L}(\Theta) = \sum_{(u,v)} \log \frac{e^{-d(u,v)}}{\sum_{v' \in neg(u)} e^{-d(u,v')}}$
- **But we perform all computations in hyperbolic space**

Backpropagation to learn embeddings

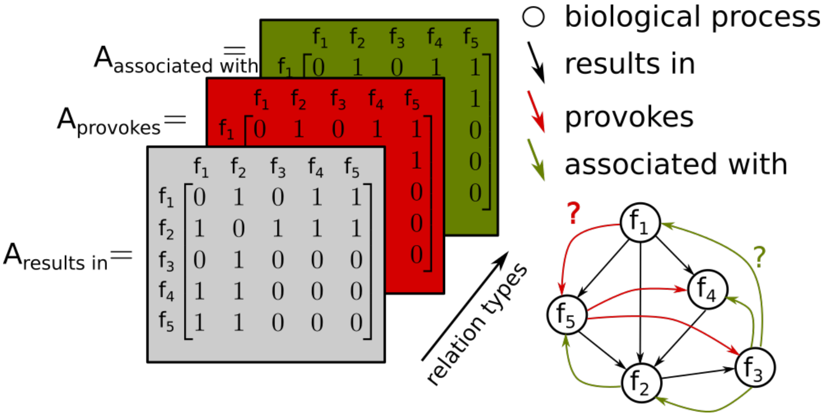


(a) Intermediate embedding after 20 epochs

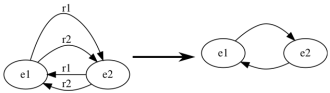
(b) Embedding after convergence

Nickel and Kiela. NIPS 2017

Link prediction for multi-relational biological knowledge graphs

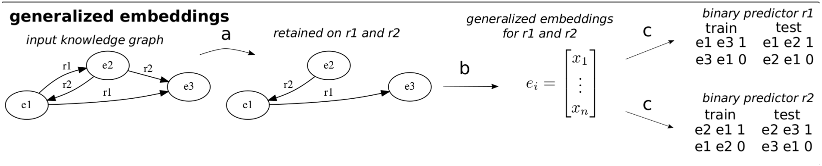


Flatenning knowledge graphs [2]



Turn KG into unlabelled directed graph, s.t., no pair of nodes is connected with more than one arc (directed edge)

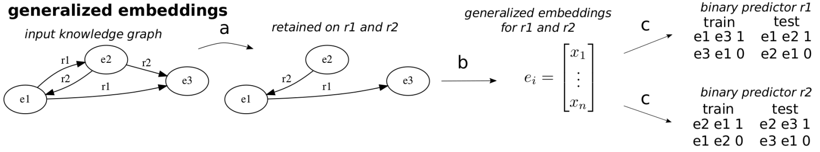
Dataset	# pairs connected with > 1 relation types
WN11	124/93003 (0.133%)
FB15-237	23700/310116 (7.642%)
UMLS	1343/6527 (20.576%)
BIO-KG	0/1619239 (0%)



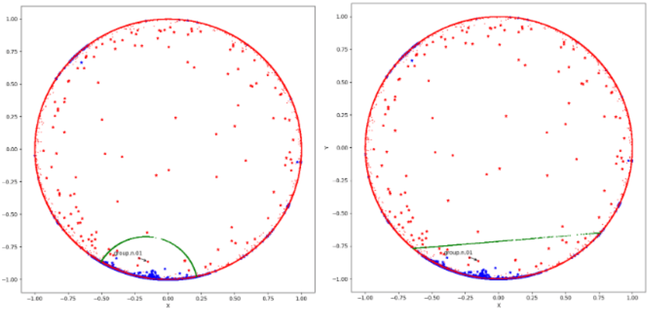
Compensate reduced information with binary classifiers fine tuned for each relation type

[2]Agibetov, Samwald. SemDeep-4@ISWC 2018

Hyperbolic Large-Margin classifier (SVM)



Agibetov, Samwald. SemDeep-4@ISWC 2018



Cho et al. arxiv 2018

Performance evaluation

Dataset	# relation types	# entities	max # links per relation type	min # links per relation type	mean # links per relation type	# pairs connected with > 1 relation types
UMLS	46	137	1021	1	142	1343/6527 (20.576%)
BIO-KG	9	346225	554366	6159	179915	0/1619239 (0%)

		Euclidean embeddings		Hyperbolic embeddings	
	dim d	Euc SVM	Hyp SVM	Euc SVM	Hyp SVM
UMLS					
	2	0.661 ± 0.023	0.616 ± 0.019	0.695 ± 0.026	$\mathbf{0.703 \pm 0.018}$
	5	$\mathbf{0.780 \pm 0.023}$	0.743 ± 0.024	0.735 ± 0.030	0.743 ± 0.024
	10	$\mathbf{0.793 \pm 0.025}$	0.754 ± 0.022	0.767 ± 0.031	0.742 ± 0.026
BIO-KG					
	2	$\mathbf{0.692 \pm 0.010}$	0.691 ± 0.010	0.613 ± 0.006	0.676 ± 0.009
	5	$\mathbf{0.776 \pm 0.010}$	0.771 ± 0.011	0.697 ± 0.008	0.756 ± 0.011
	10	0.732 ± 0.009	0.723 ± 0.008	0.711 ± 0.010	$\mathbf{0.763 \pm 0.010}$

Lessons learned

Benefit of learning hyperbolic embeddings

- fewer dimensions to capture latent semantic and hierarchical information
- scalability and interpretability (easier to visualize 2 or 3 dimensions)

From our preliminary results

- hyperbolic embeddings learn hierarchical relationships in UMLS better than Euclidean embeddings (lower dimensions)
- For complex and big graphs (BIO-KG) train hyperbolic embeddings for longer periods ($>$ 500 epochs)

Open issues and future directions

- even with recent advances in Riemannian SGD optimization [3], learning hyperbolic embeddings still much slower than in the Euclidean case
- next steps should be focused on end-to-end hyperbolic embedding training (hyperbolic large-margin classifier loss is directly incorporated during the training process)
- code available at `https://github.com/plumdeq/hsvm`
- contact: `asan.agibetov@meduniwien.ac.at`

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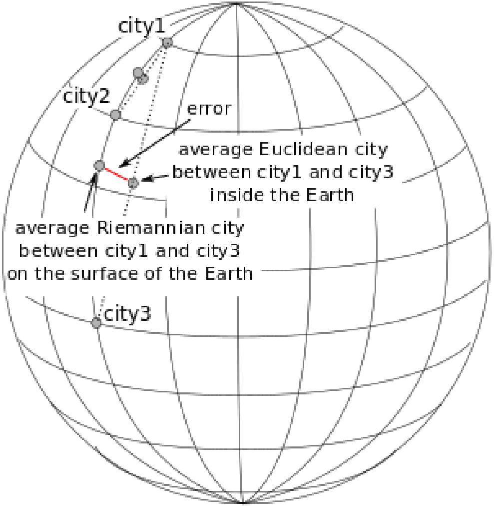
[3] "Gradient descent in hyperbolic space". Wilson and Leimeister, 2018

Why non-Euclidean space - (low-dim) manifolds

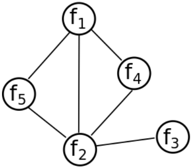
- Computing on a lower dimensional space leads to manipulating fewer degrees of freedom
- Non-linear degrees of freedom often make more intuitive sense
    - cities on the earth are better localized giving their longitude and latitude (2 dimensions)
    - instead of giving their position x, y, z in the Euclidean 3D space



Learning graph embeddings

- Learn *link estimate* $Q(u, v) \mapsto [0, 1]$ (u, v node pairs) and approximate graph structure (connectivity) with MLE (maximum likelihood estimation)[4]
  - $Pr(G) = \prod_{(u,v)\in E_{train}} Q(u, v) \prod_{(u,v)\notin E_{train}} 1 - Q(u, v)$

- If Q perfect estimator then $Pr(x) = 1$ iff $x = G$ (i.e., graph can be fully reconstructed)
- Q can be *trained* to estimate links at different *orders*, i.e., approximate A^n.



1-order paths

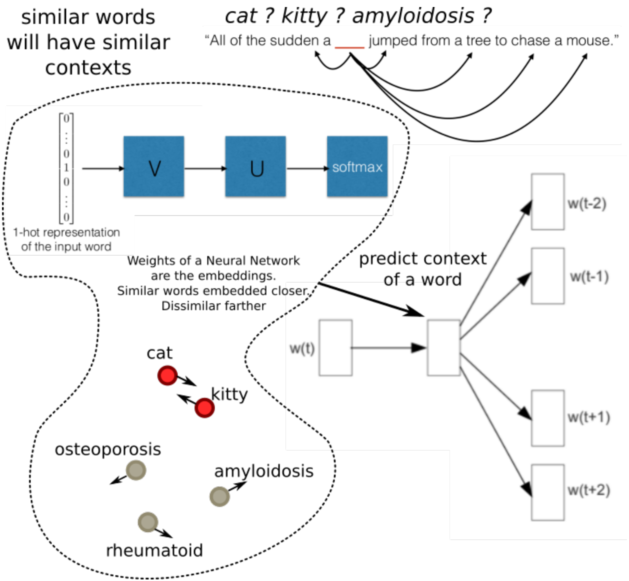
$$A = \begin{array}{c} \\ f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \end{array} \begin{array}{c} \begin{array}{ccccc} f_1 & f_2 & f_3 & f_4 & f_5 \end{array} \\ \begin{bmatrix} 0 & 1 & 0 & 1 & 1 \\ 1 & 0 & 1 & 1 & 1 \\ 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \end{bmatrix} \end{array}$$

2-order paths

$$A(A) = A^2 = \begin{array}{c} \\ f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \end{array} \begin{array}{c} \begin{array}{ccccc} f_1 & f_2 & f_3 & f_4 & f_5 \end{array} \\ \begin{bmatrix} 3 & 2 & 1 & 1 & 1 \\ 2 & 4 & 0 & 1 & 1 \\ 1 & 0 & 1 & 1 & 1 \\ 1 & 1 & 1 & 2 & 2 \\ 1 & 1 & 1 & 2 & 2 \end{bmatrix} \end{array}$$

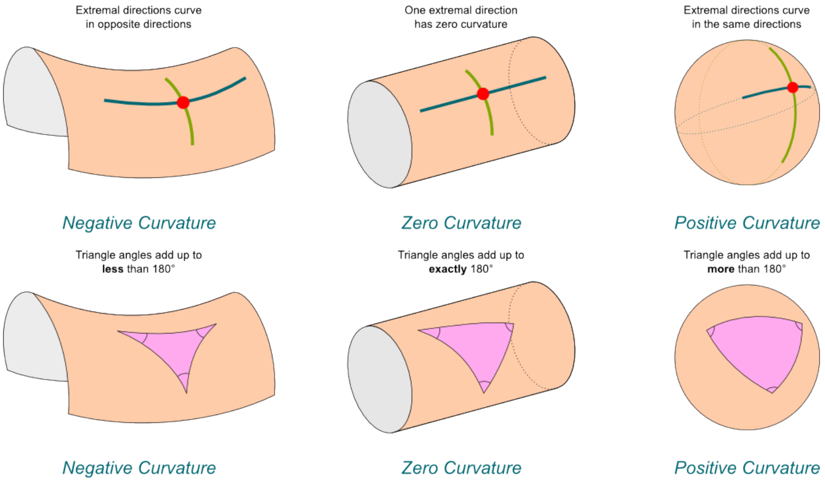
[4] "Graph likelihood", Haija, ... Perozzi, ..., CIKM17, NeurIPS 2018

Similar principle as word2vec [5]

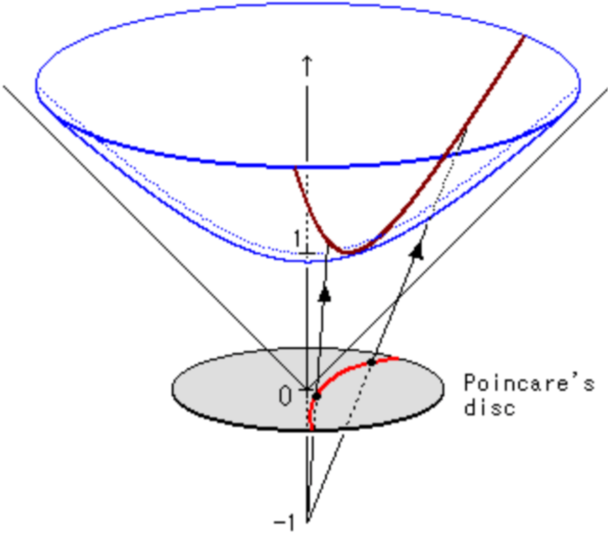


[5] "word2vec", Mikolov et al., NIPS 2014

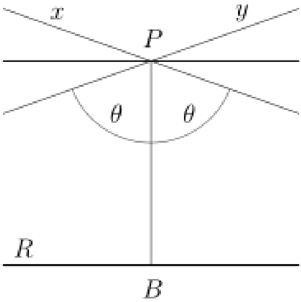
What's so special about Riemannian geometry - curvature

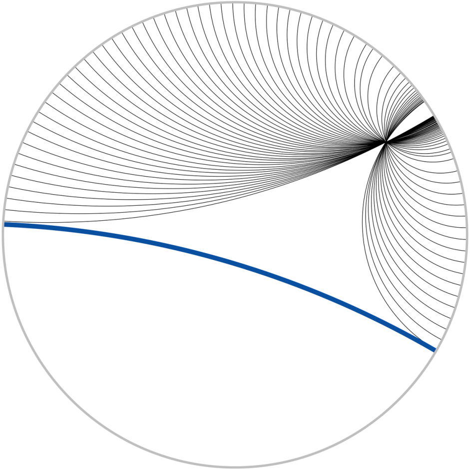


Model of hyperbolic geometry

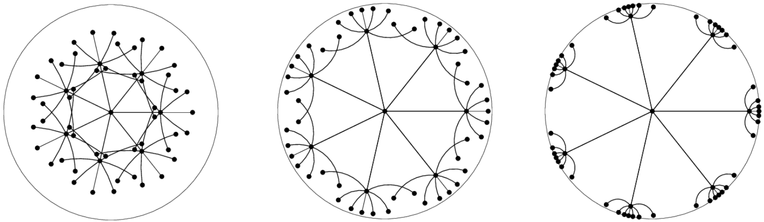


Properties of hyperbolic geometry

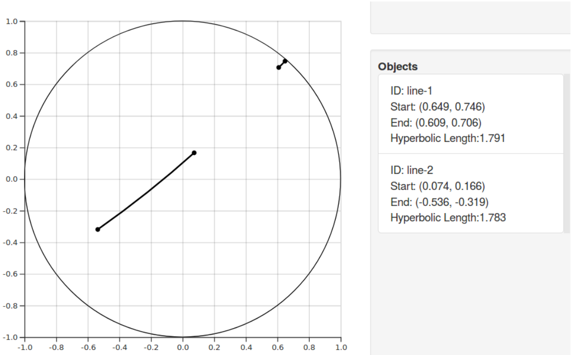




Computing lengths in hyperbolic geometry



Radius 1 Radius 2 Radius 3



Approximation of graph distance