Mining Networks

Chapter 6 — Graph Embeddings

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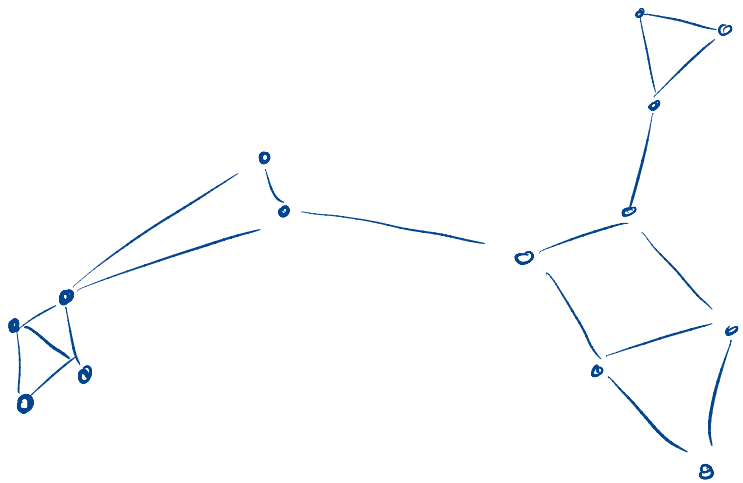
Overview

1. Problem Formalization
2. Techniques
3. Unsupervised Benchmark
4. A Few Applications
5. Experiments

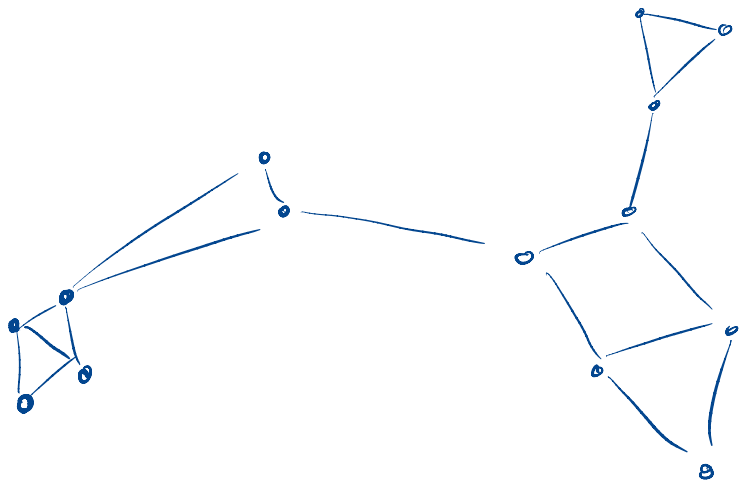
Introduction

To extract useful structural information from graphs, it is convenient to embed it in a geometric space by assigning coordinates to each node.



Introduction

Classical embeddings: nearby nodes are more likely to share an edge than those far from each other, or are similar in some sense.



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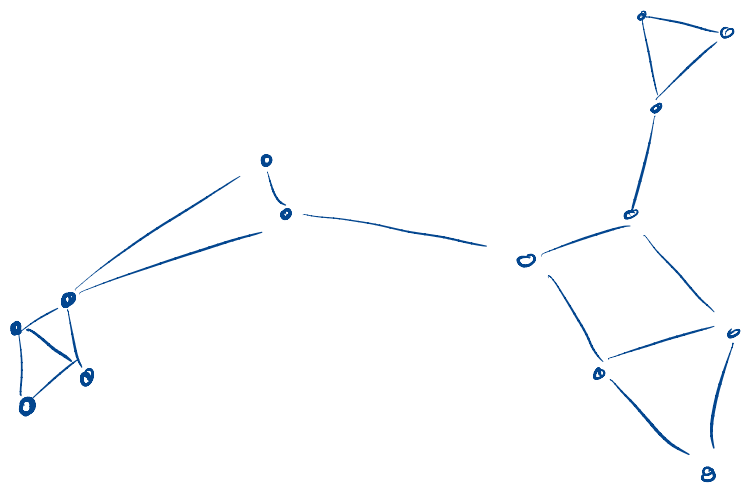
Structural embeddings: nodes with similar structure of their local ego-nets should be embedded close to each other.



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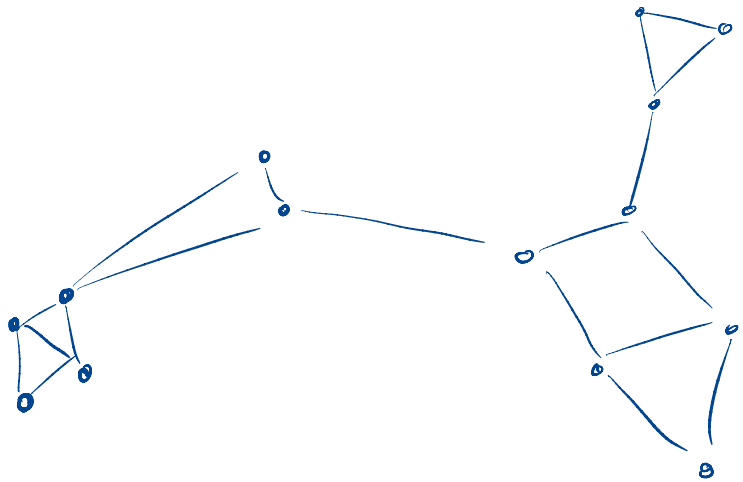

There are many applications, including:

– Node Classification (say, bot detection): structural,

– Node Clustering and Community Detection: classical,

– Link Prediction and Missing Links: classical,

– Visualization.

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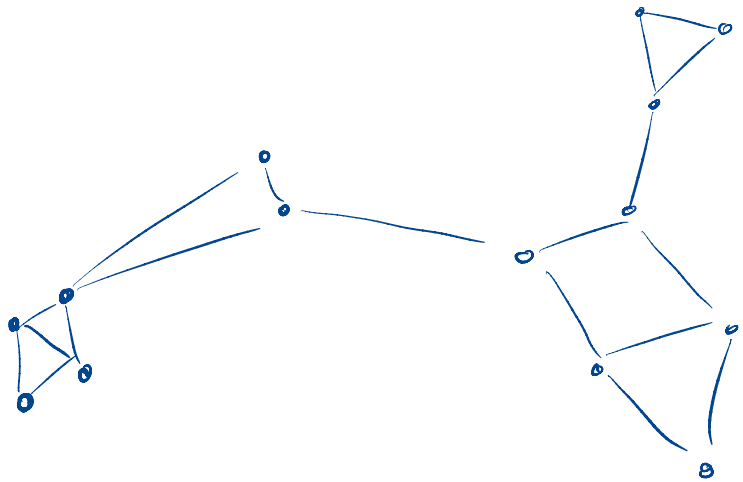

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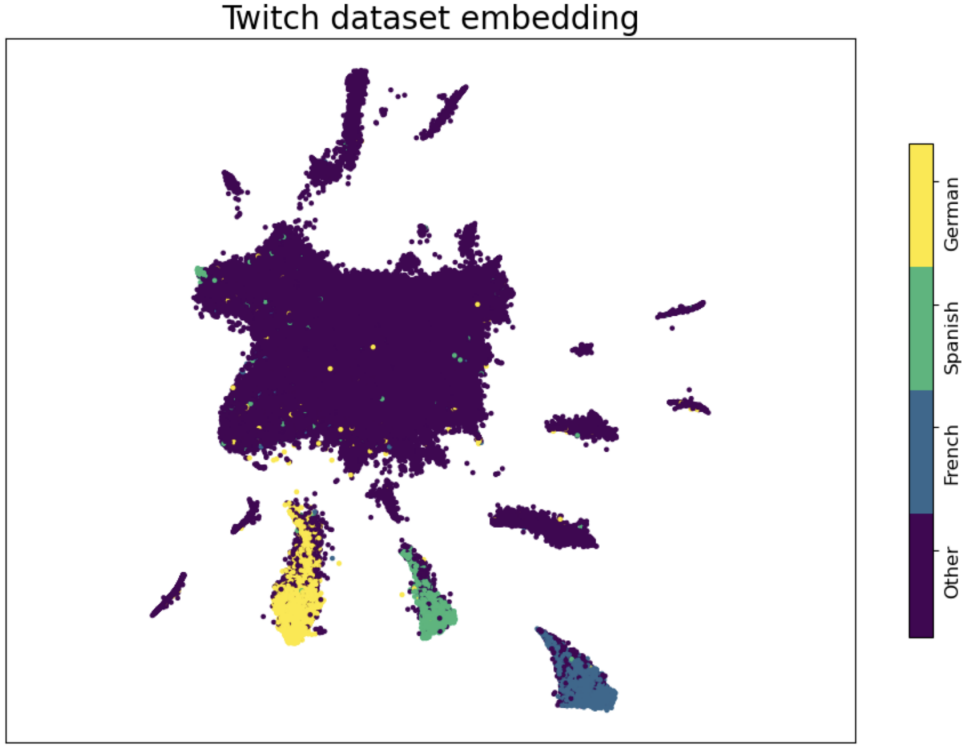
Drawback: graph embedding often requires domain experts.

Illustration

Twitch gamers social network:

– 168,114 nodes representing users

– 6,797,557 (undirected) edges — mutual followers

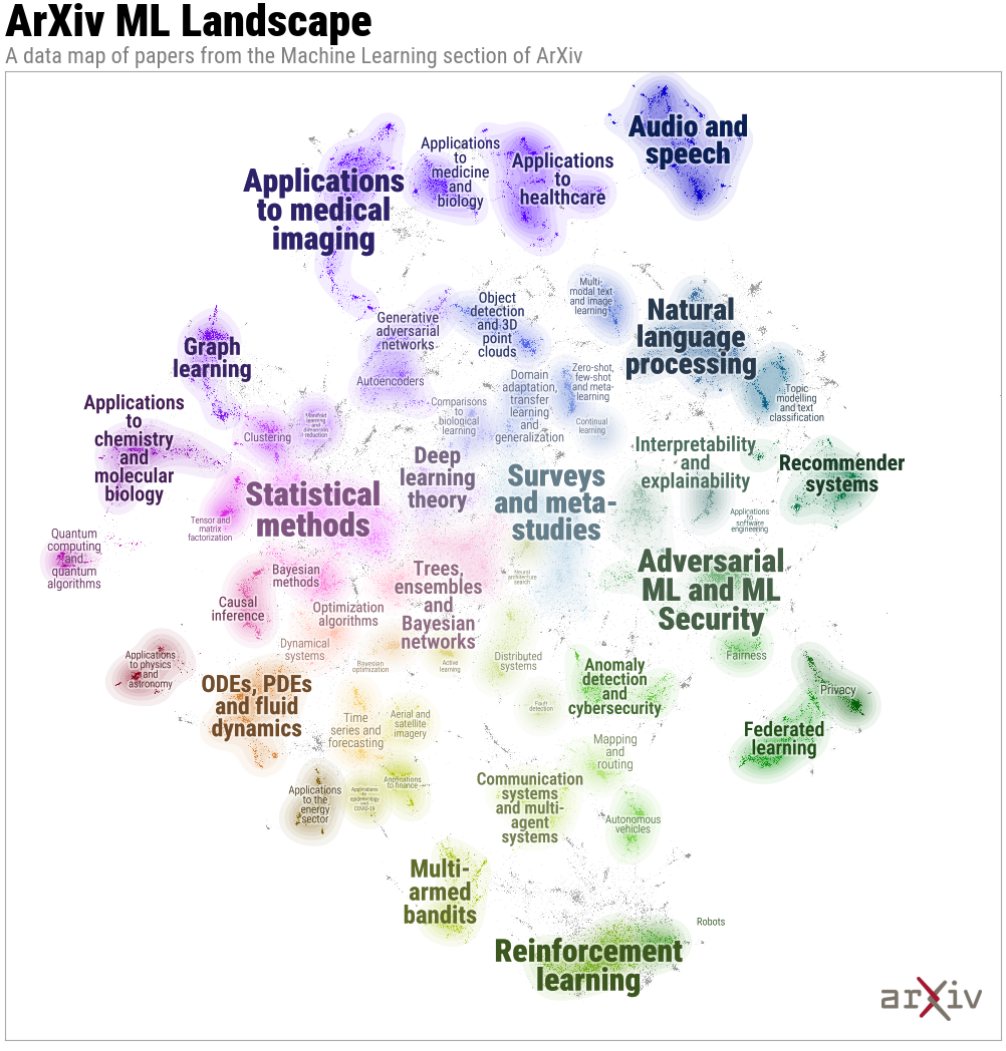


Node2Vec + UMAP

Illustration

ArXiv ML Landscape

(Example of DataMapPlot in action)



Problem Formalization

Embedding

$G = (V, E)$ — weighted undirected graph on the set of nodes $V = \{v_1, v_2, \ldots, v_n\}$. (We will discuss directed graphs later on.)

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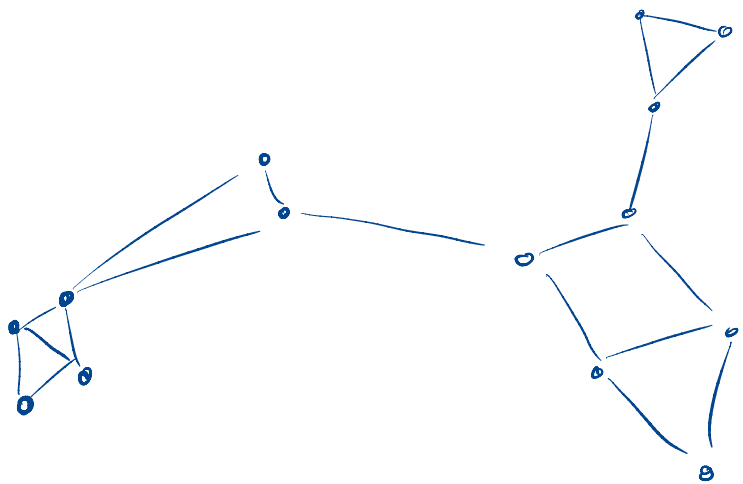
Embedding — function $\mathcal{E} \colon V \to \mathbb{R}^k$; k is much smaller than n.



Algorithms Based on Random Walk

These methods are inspired by the Word2Vec algorithm for word embedding in Natural Language Processing (NLP).

Main idea: words are known by the company they keep.

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"Graph *embedding maps* **nodes** *to vector* space".

The model is trained to predict the words in *italics* given the word "**nodes**" as input.

Algorithms Based on Random Walk

Similarly to HOPE, SkipGram associates two embeddings with each word: $\mathbf{E}_s$ ("source") and $\mathbf{E}_t$ ("target").

They try to capture relationships between the input words and the words that they aim to predict and vice versa.

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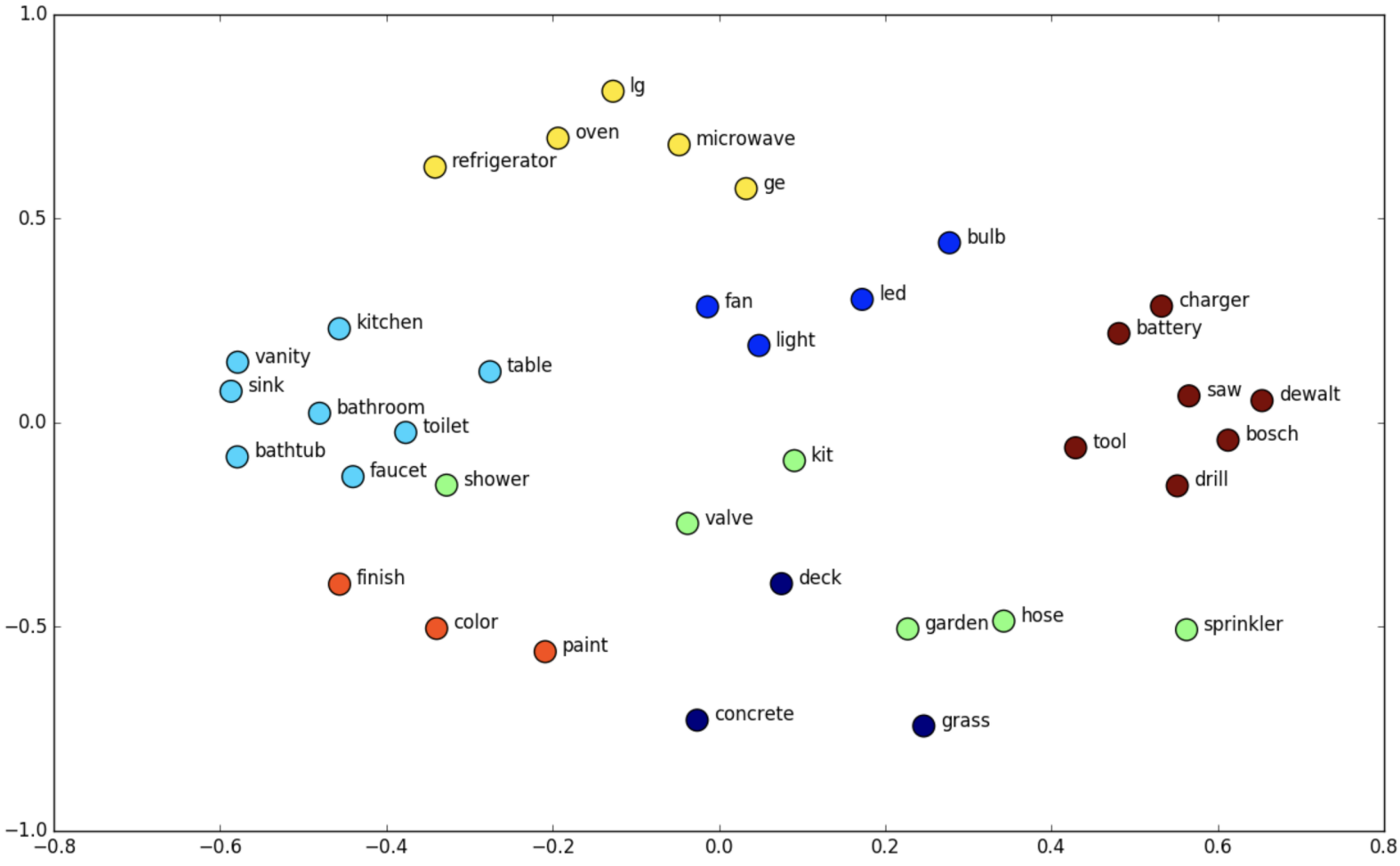
Given a word i, the probability $p_{i,j}$ that we see word j in its neighbourhood is approximated by the softmax function:

$$q_{i,j} = \frac{\exp(e_{t,j}^T e_{s,i})}{\sum_{\ell=1}^{|W|} \exp(e_{t,\ell}^T e_{s,i})}.$$

The model is trained using maximum likelihood estimation.

Algorithms Based on Random Walk



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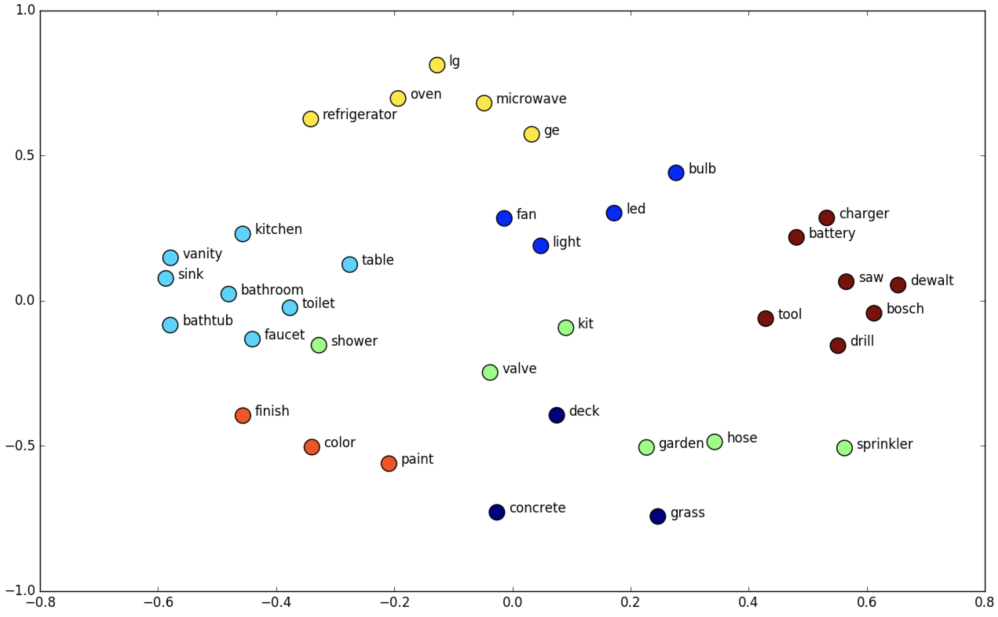


Unsupervised learning (no syntactic or semantic relationships among words are provided).

Yet, word embeddings seem to capture these relationships!

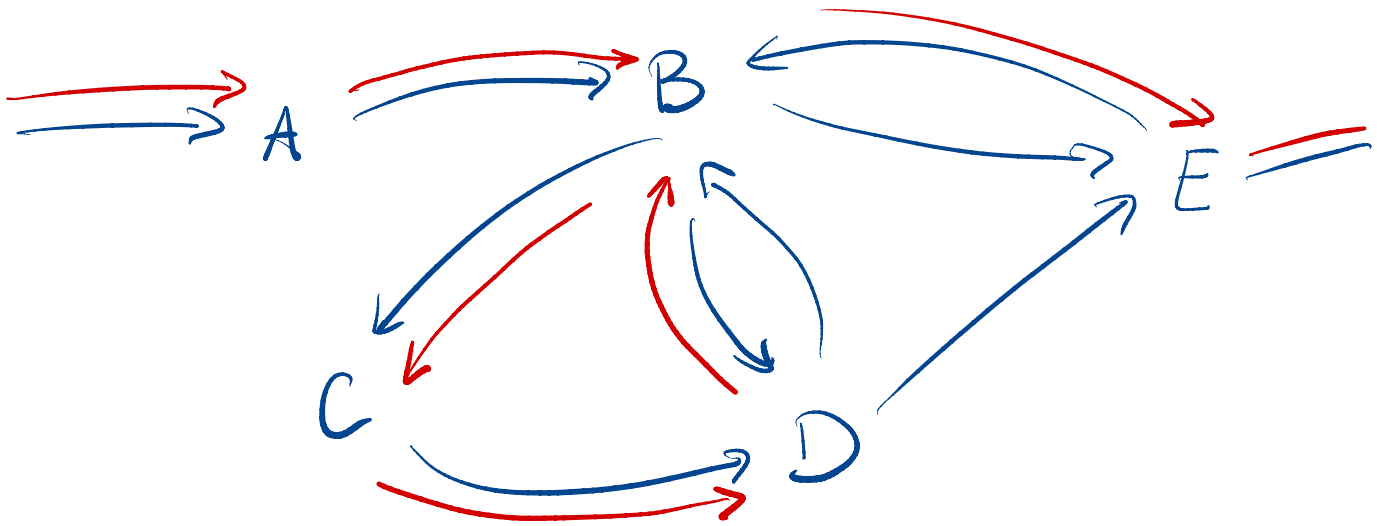
king - man + woman ≈ queen

Paris - France + Germany ≈ Berlin

Algorithms Based on Random Walk

Generalization to graphs.

– the words are simply the nodes of a graph,
– sentences (sequences of nodes) are generated via random walks on a graph (exact procedure depends on the algorithm).

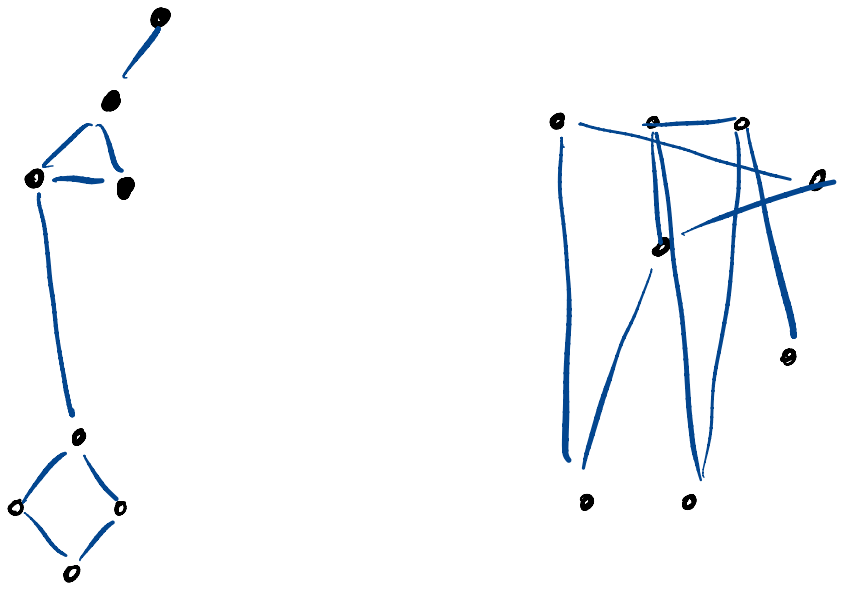


Unsupervised Benchmark

Main Goal

There are many embedding algorithms (techniques from linear algebra, random walks, or deep learning) and the list grows.

Results vary a lot.



How can we evaluate these embeddings? Which one is the best and should be used? Important question: GIGO.

Big Picture

Input: Graph $G = (V, E)$ on n nodes with the degree distribution $\mathbf{w} = (w_1, \ldots, w_n)$.

Embedding of nodes of V, $\mathscr{E} : V \to \mathbb{R}^k$ (typically many).

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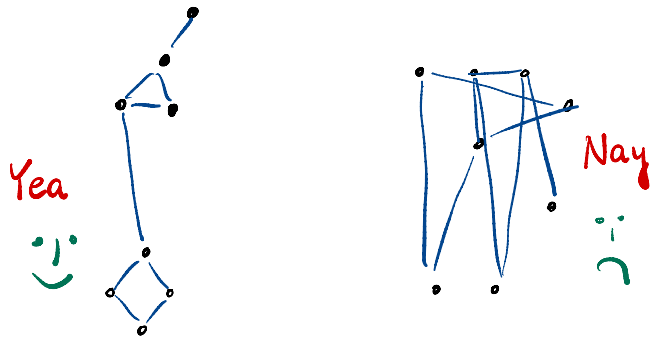
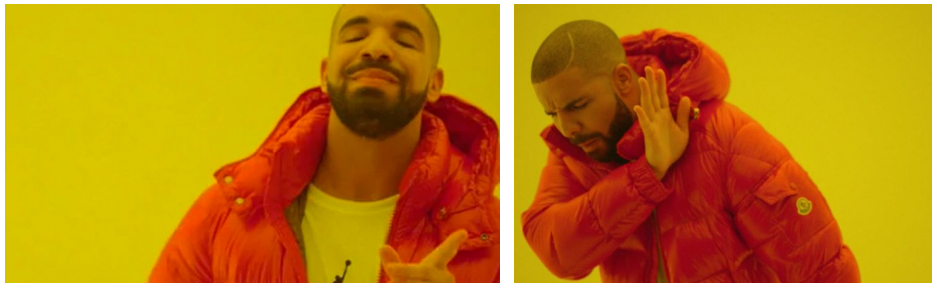
Output: two "divergence scores" (global and local) assigned to $\mathscr{E}$ (smaller is better).





Global Score

Global score:

– looks at the network and the associated embeddings “from the distance”;

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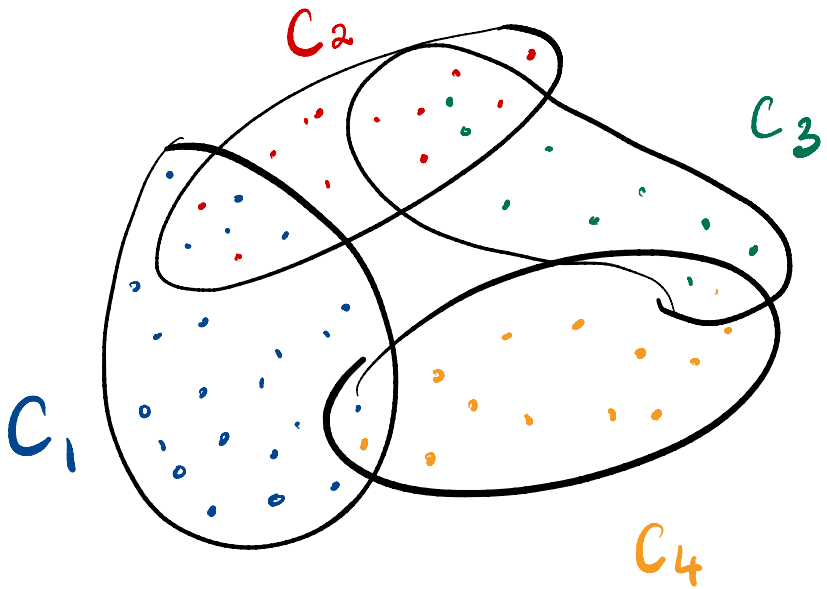
– looks at the network and the associated embeddings "from the distance";
– evaluates the embeddings based on their ability to capture global properties of the network, namely, edge densities;

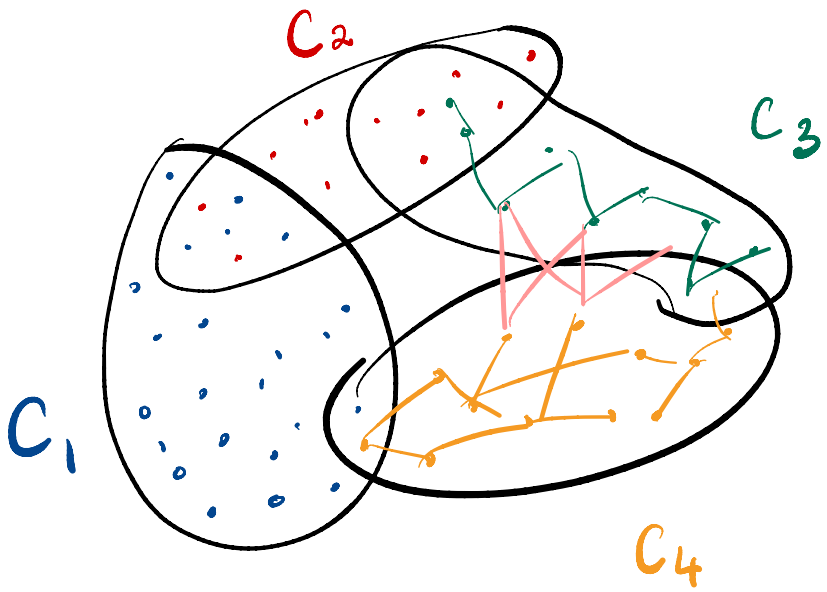
– goodness-of-fit test for the provided embedding, rather than simply checking its predictive power—its aim is similar to the well-known Hosmer–Lemeshow test for logistic regression (used frequently in risk prediction models).

Global Score



Step 1: Run some graph clustering algorithm to obtain a partition of V into ℓ communities $C_1, \ldots, C_\ell$.

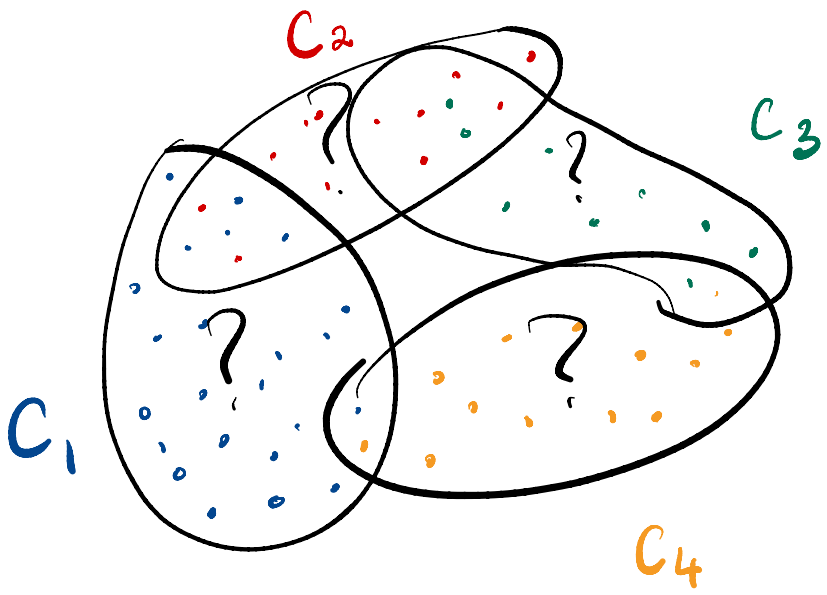
Global Score



Step 2: Compute $c_{i,j}$ (including $j = i$): proportion of edges with one endpoint in C_i and the other one in C_j.

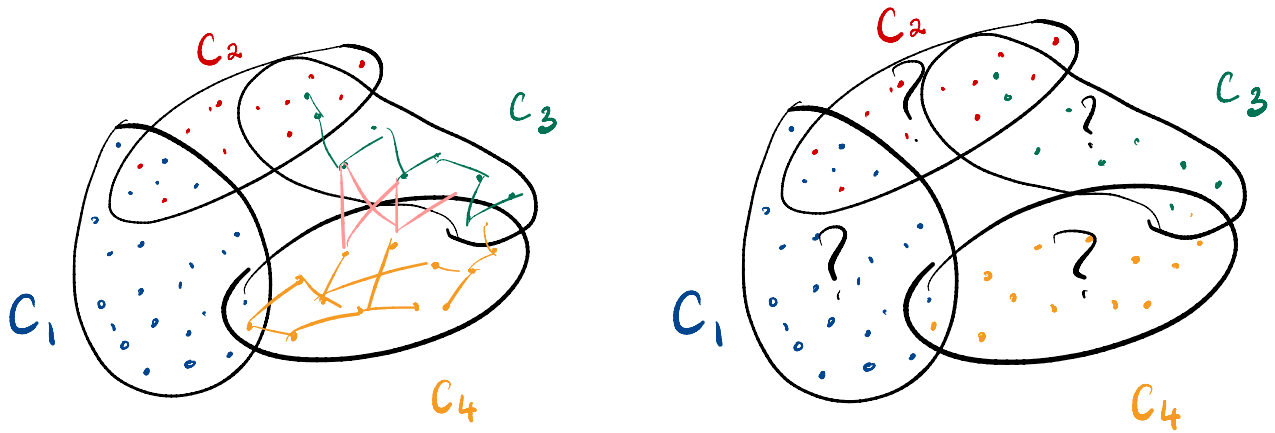
Note that we do not use $\mathscr{E}$.

Global Score



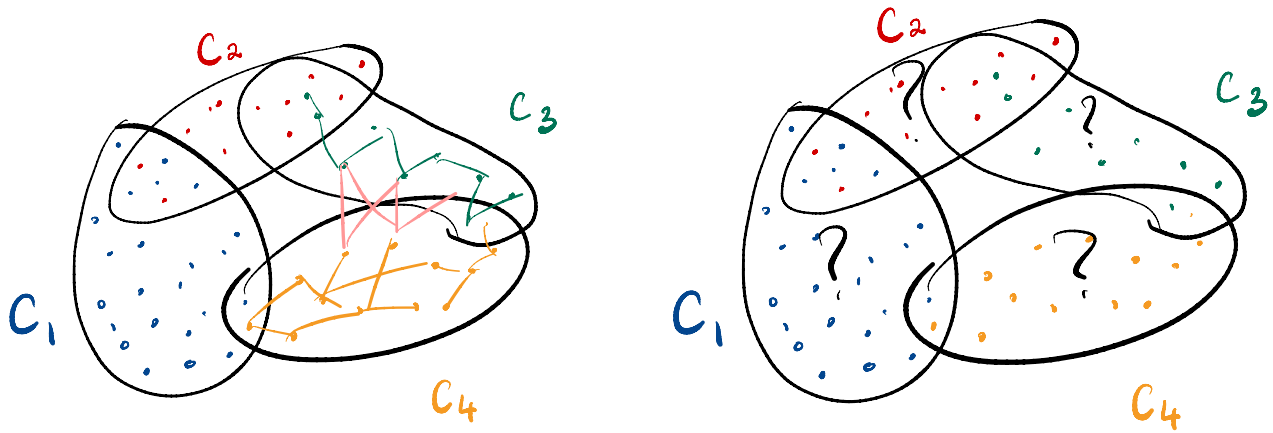
Step 3: Compute $b_{i,j}$ (including $j = i$): the expected proportion of edges with one endpoint in C_i and the other one in C_j, in the geometric Chung-Lu model $\mathcal{G}(\mathbf{w}, \mathcal{E}, \alpha)$.
Note that we do not use G, only $\mathbf{w}$ (on top of $\mathcal{E}$ and parameter α, the "aversion" for long links).

Global Score



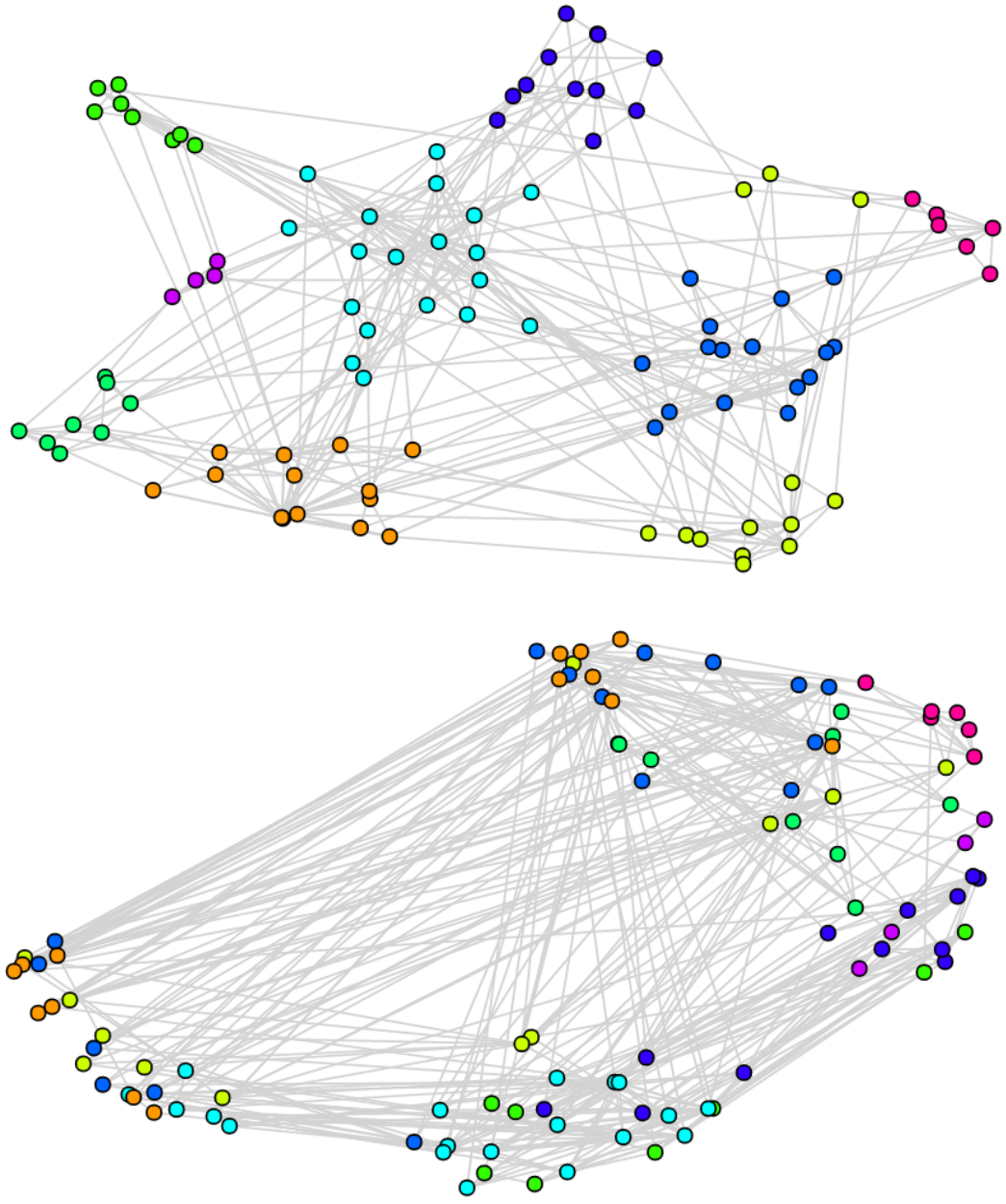
Step 4: Compute Δ_α: the Jensen-Shannon divergence between the two vectors (smoothed version of the Kullback-Leibler divergence we mentioned earlier).

Global Score

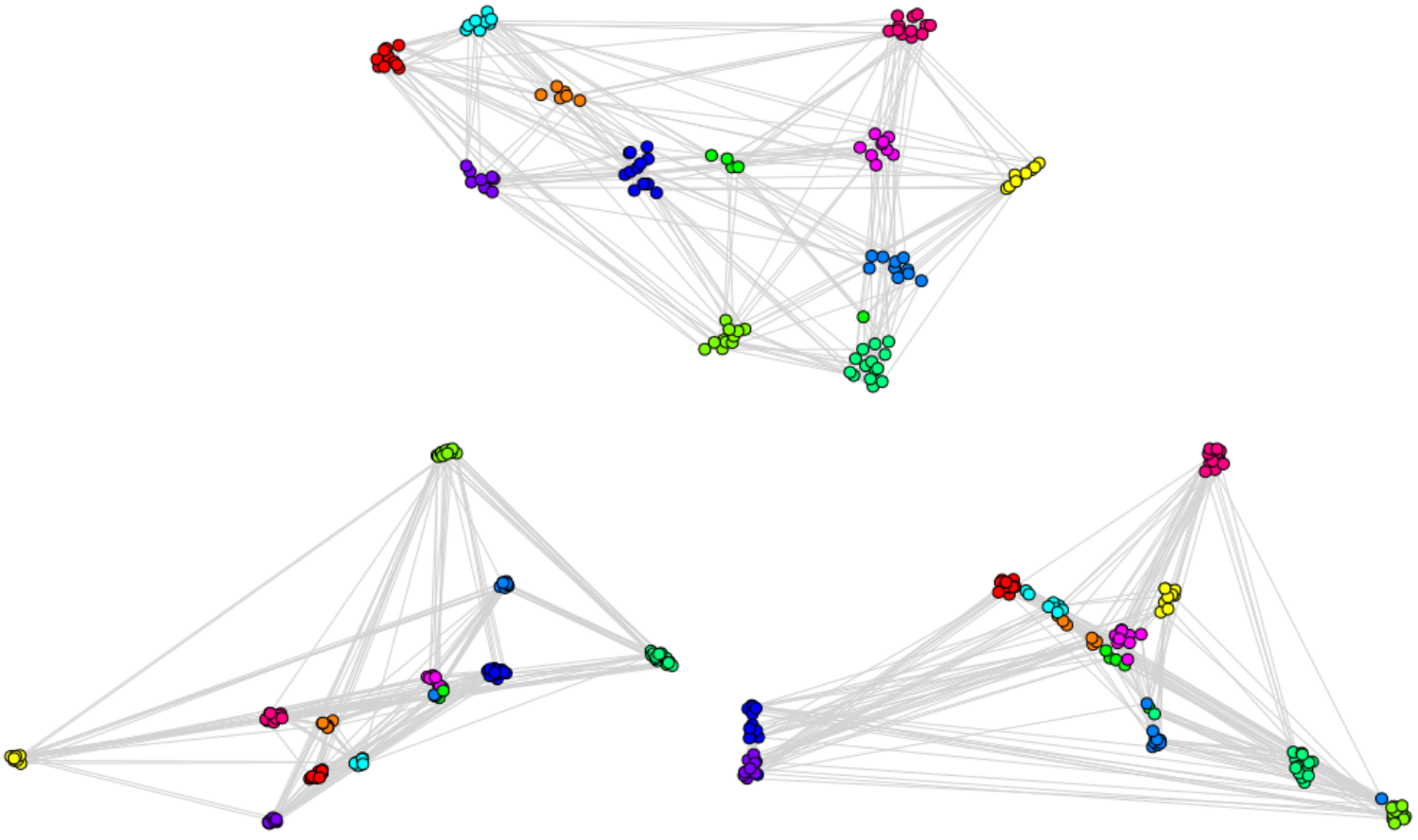


Step 5: Take the minimum Δ_α over various choices for parameter α that measures the "aversion" for long links. It defines the global score.

The worst and the best LFR graph ($\mu = 0.35$)



The worst and the best College Football graph



Local Score

Local score:

– provides a complementary test,

– looks at the network and embeddings "under the microscope", trying to see if a local structure of a graph is well reflected by the associated embedding.

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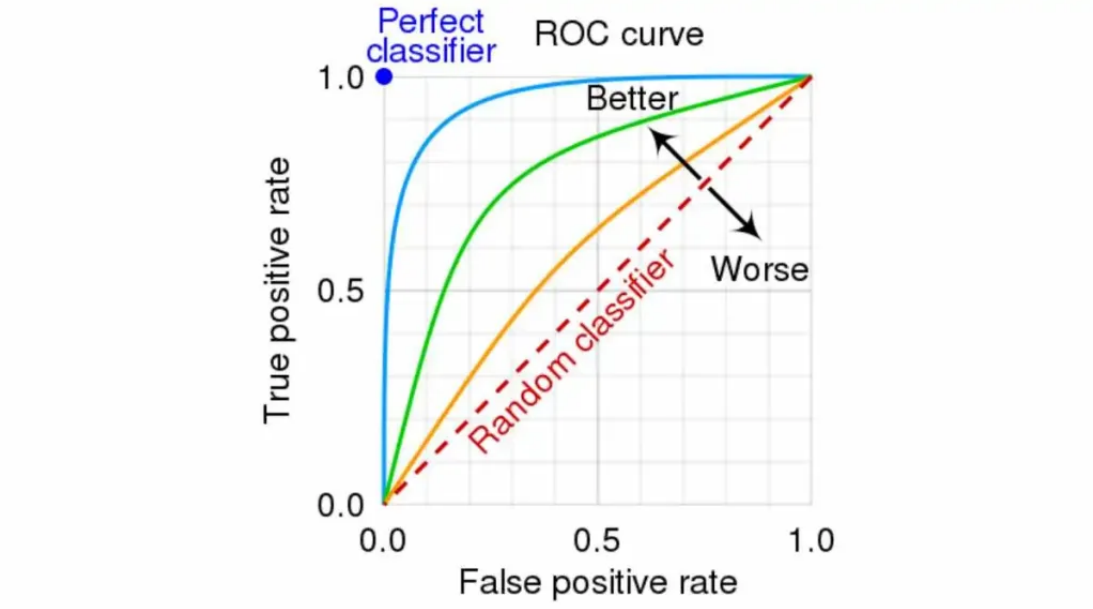
– S^+ and S^-: edges and non-edges,
– $p(u, v)$: the probability of an edge uv to be present in the geometric Chung-Lu model $\mathcal{G}(\mathbf{w}, \mathcal{E}, \alpha)$,
– build a binary classifier to see if $p(u, v)$ can be used to distinguish edges from non-edges.

Local Score

– The ROC (Receiver Operating Characteristic) is a curve showing the performance of a classification model at all classification thresholds.

y-axis: True Positive Rate (Sensitivity) — the proportion of actual positive instances the model correctly identifies

x-axis: False Positive Rate (1-Specificity) — the proportion of actual negative instances incorrectly classified as positive



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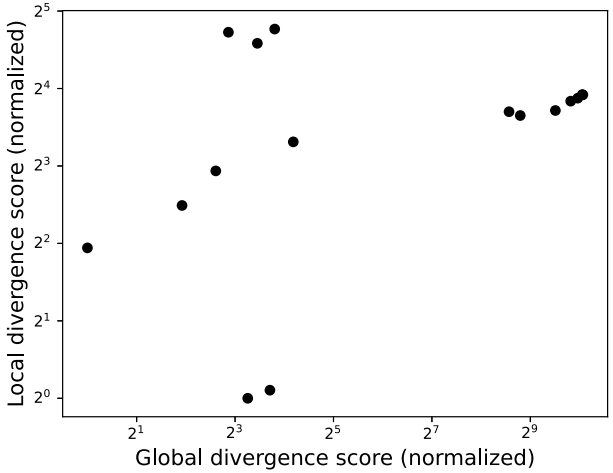
$$\frac{\sum_{st \in S^+} \sum_{uv \in S^-} 1\{p(s,t) > p(u,v)\}}{|S^+| \cdot |S^-|}.$$

(Can be easily approximated by sampling.)

Example: ABCD (3 communities)



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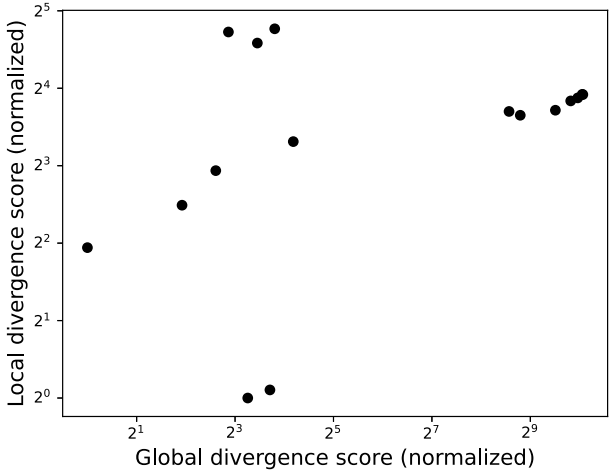
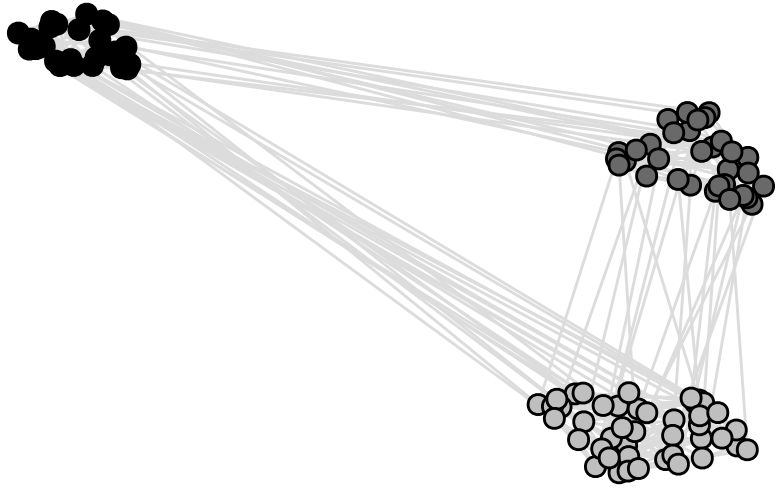


Low global divergence



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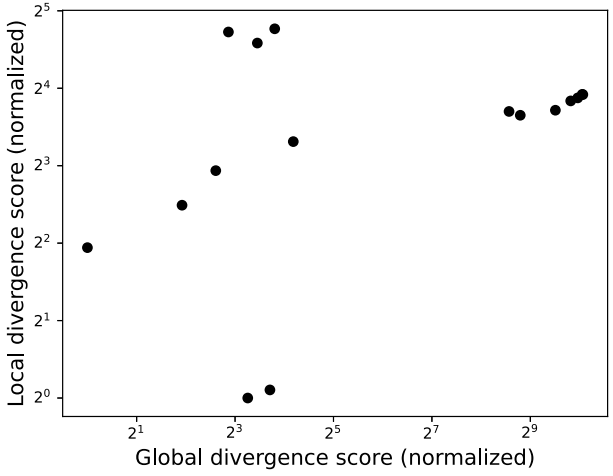

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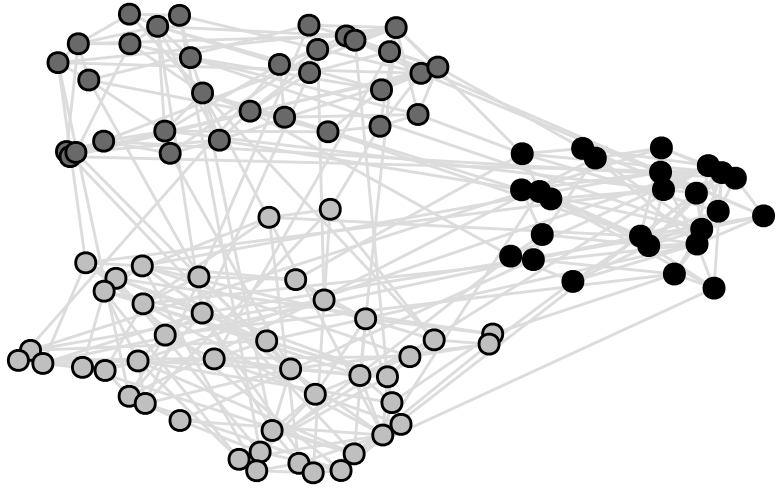

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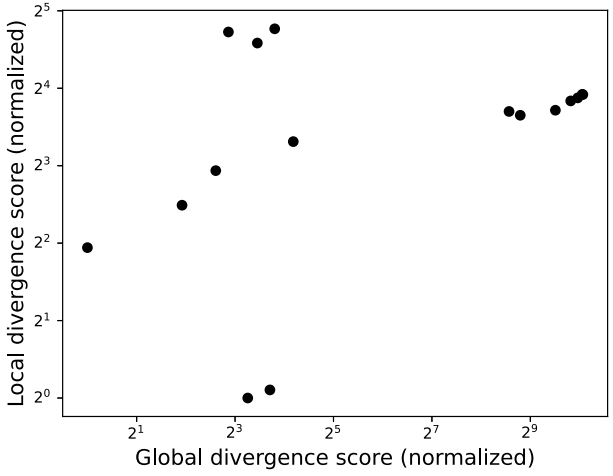
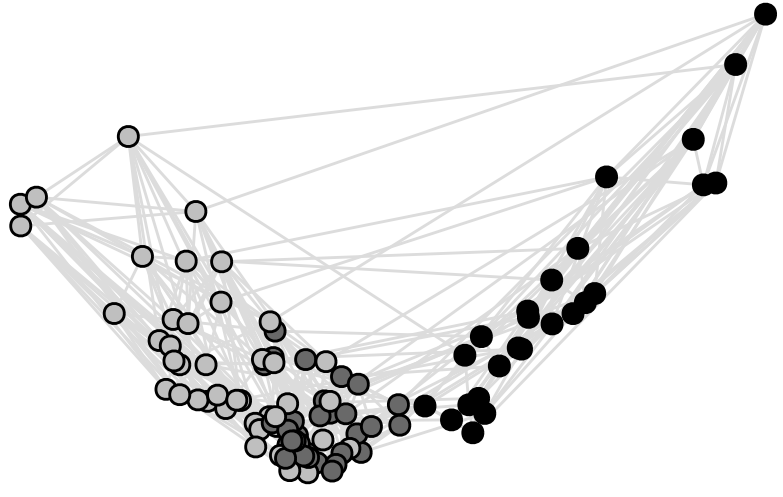


Both divergences high



Geometric Chung-Lu model

We generalized the Chung-Lu model:

$$p_{i,j} = x_i x_j g(d_{i,j}),$$

where $d_{i,j} = \text{dist}(\mathscr{E}(v_i), \mathscr{E}(v_j))$ and $g(x) = g_\alpha(x)$ is some decreasing (similarity) function such as

$$g(d) = \left(1 - \frac{d - d_{\min}}{d_{\max} - d_{\min}}\right)^\alpha,$$

where $d_{\min}$ and $d_{\max}$ are the minimum, and respectively the maximum, distance between nodes in embedding $\mathscr{E}$.

Geometric Chung-Lu model

x_i's have to be tuned so that $\mathbb{E}[\deg(v_i)] = w_i$.

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We propose scalable (approximation) algorithm with running time $O(n \ln n)$.

THE END