

Mining Networks

Chapter 6 — Graph Embeddings

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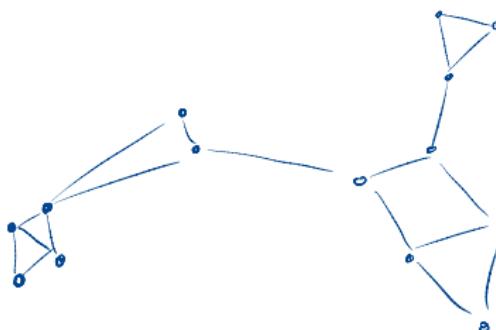


Overview

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

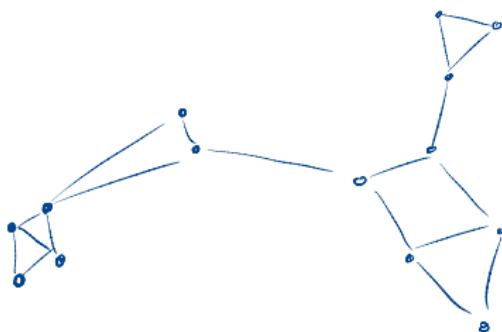
Introduction

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



Introduction

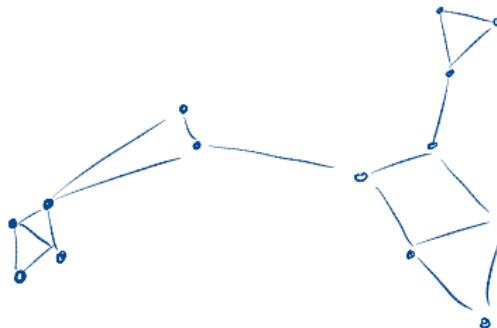
Classical embeddings: nearby nodes are more likely to share an edge than those far from each other, or are similar in some sense.



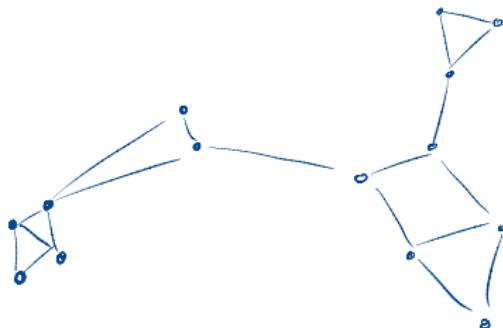
Introduction

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

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



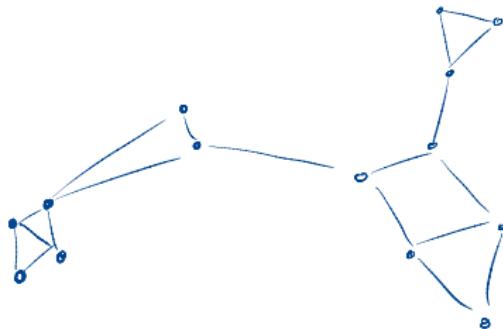
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There are many **applications**, including:

- Node Classification (say, bot detection): **structural**,
- Node Clustering and Community Detection: **classical**,
- Link Prediction and Missing Links: **classical**,
- Visualization.

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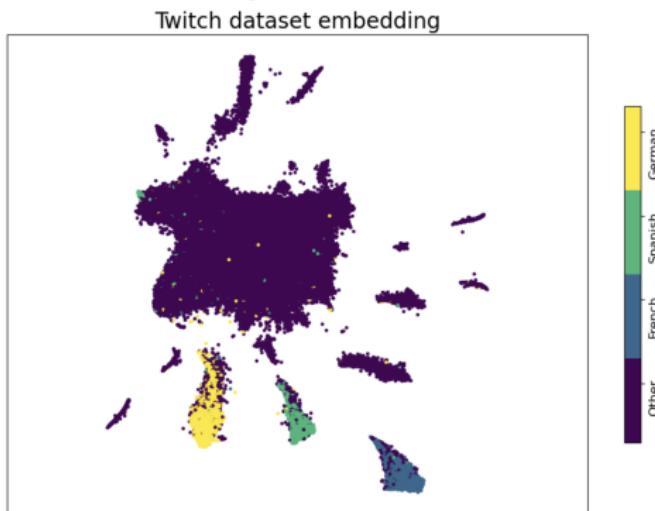
- Node Classification (say, bot detection): **structural**,
- Node Clustering and Community Detection: **classical**,
- Link Prediction and Missing Links: **classical**,
- Visualization.

Drawback: graph embedding often requires domain experts.

Illustration

Twitch gamers social network:

- 168,114 nodes representing users
- 6,797,557 (undirected) edges — mutual followers

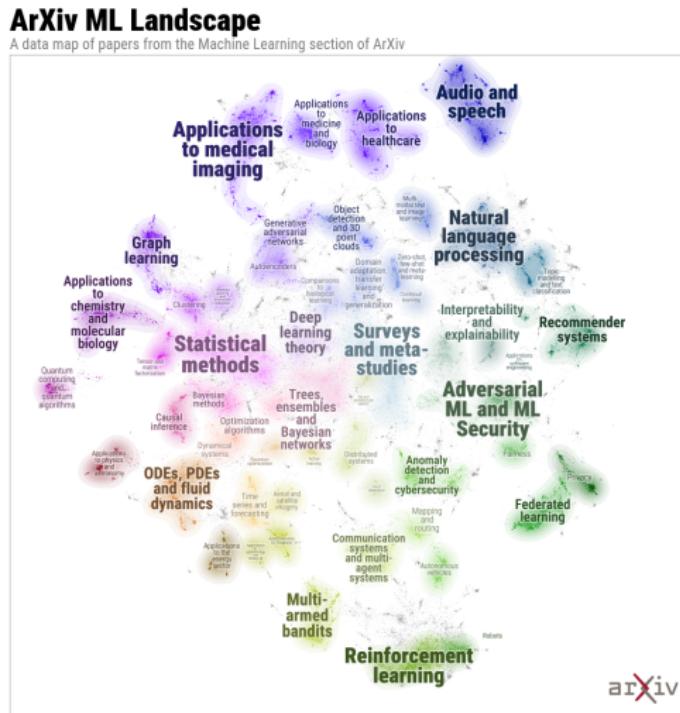


Node2Vec + UMAP

Illustration

ArXiv ML Landscape

(Example of DataMapPlot in action)



Problem Formalization

Embedding

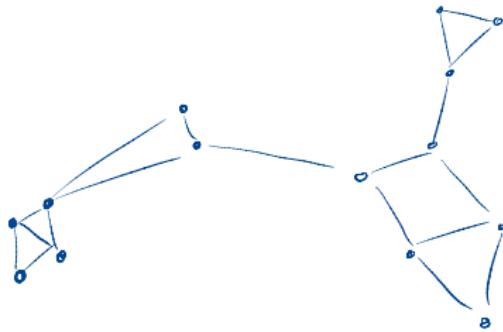
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 $V = \{v_1, v_2, \dots, v_n\}$. (We will discuss **directed** graphs later on.)

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



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There are a few natural **proximity measures**, each produces a matrix $\mathbf{S} = (s(v_i, v_j))_{i,j \in [n]}$.

$s(v_i, v_j) \in \mathbb{R}_+ \cup \{0\}$ — proximity between nodes v_i and v_j .

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It is desired that matrix \mathbf{S} is **symmetric** but not all proximity measures guarantee this property. (Embedding algorithm has to deal with asymmetric matrices if needed.)

The **diagonal** of \mathbf{S} is usually **ignored** by embedding algorithms but it does not have to be.

First-order Proximity

Two nodes are simply more **similar** if they are connected by an **edge** with **larger weight**.

First-order Proximity

The **first-order proximity** $s_1(v_i, v_j)$ is the weight of the edge $v_i v_j$, that is, $s_1(v_i, v_j) = a(v_i, v_j)$, where $\mathbf{A} = (a(v_i, v_j))_{i,j \in [n]}$ is the **adjacency matrix**.

Second-order Proximity

It measures the similarity between the **neighbourhoods**.

Second-order Proximity

The **second-order proximity** $s_2(v_i, v_j)$ is a similarity between v_i 's neighbourhood

$$s_1(v_i) = (s_1(v_i, v_1), s_1(v_i, v_2), \dots, s_1(v_i, v_n))$$

and v_j 's neighbourhood

$$s_1(v_j) = (s_1(v_j, v_1), s_1(v_j, v_2), \dots, s_1(v_j, v_n)).$$

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The **second-order proximity** $s_2(v_i, v_j)$ is a similarity between v_i 's neighbourhood and v_j 's neighbourhood.

The **cosine similarity**, a standard measure of similarity, is defined as the **cosine** of the **angle** between them:

$$s_2(v_i, v_j) = \frac{\sum_{\ell=1}^n s_1(v_i, v_\ell) s_1(v_j, v_\ell)}{\sqrt{\sum_{\ell=1}^n s_1(v_i, v_\ell)^2} \sqrt{\sum_{\ell=1}^n s_1(v_j, v_\ell)^2}}.$$

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Generalization: for any $k \in \mathbb{N} \setminus \{1, 2\}$, the **k th-order proximity** $s_k(v_i, v_j)$ is the similarity between v_i 's $(k - 1)$ st neighbourhood $s_{k-1}(v_i)$ and v_j 's $(k - 1)$ st neighbourhood $s_{k-1}(v_j)$.

Katz Index

Alternatively, one may want to use some centrality measure such as the **Katz centrality**. It tries to capture the **relative influence** of a node within a network by considering **walks** of any length but **penalize longer walks** by introducing the **attenuation factor α** .

Katz Index

Fix any α such that $0 < \alpha < \min\{1, 1/|\lambda|\}$, where λ is the leading eigenvalue of adjacency matrix \mathbf{A} . The **Katz Index** $\mathbf{S}_\alpha^{\text{Katz}}$ is defined as follows:

$$\mathbf{S}_\alpha^{\text{Katz}} = \sum_{i=1}^{\infty} (\alpha \cdot \mathbf{A})^i = (\mathbf{I}/\alpha - \mathbf{A})^{-1} \mathbf{A}.$$

Personalized PageRank

This variant (commonly used by web search engines) of the well-known **PageRank** depends on two parameters: the **jumping constant** α and the **seed** node $s \in V$.

Random walk continues with probability α and goes back to the **seed node** s with probability $1 - \alpha$.

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where the **auxiliary** matrix $\hat{\mathbf{A}}$ is defined as in **PageRank**.

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$\mathbf{S}_\alpha^{\text{PPR}}$ is usually **not** symmetric.

Common Neighbours

In the next definition, we simply **count** the number of nodes that have both v_i and v_j as their neighbours.

Common Neighbours

Given adjacency matrix \mathbf{A} , the **Common Neighbours** \mathbf{S}^{CN} is defined as follows:

$$\mathbf{S}^{\text{CN}} = \mathbf{A}^2.$$

Recall that: \mathbf{A}^k is equal to the **number of walks of length k** from node v_i to node v_j .

Adamic-Adar

Variant of the **common neighbours** in which the fact that two nodes are **common neighbours** of some node with **very large neighbourhood** is less significant.

Adamic-Adar

The **Adamic-Adar** \mathbf{S}^{AA} is defined as follows:

$$s^{AA}(v_i, v_j) = \sum_{v_k \in N(v_i) \cap N(v_j)} \frac{1}{\ln(\deg(v_k))},$$

for $i \neq j$ and $s^{AA}(v_i, v_i) = 0$.

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If this happens, then we have two options:

- ignore it and let the embedding algorithm to deal with this (for example, LLE and HOPE can do it),
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There are also some proximity measures (for example, SimRank that is similar to second-order measures) that can be explicitly used to compute \mathbf{S} for directed graphs.

Techniques

Linear Algebra Algorithms

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$$\hat{a}(u, v) = a(u, v)/\deg^{out}(u).$$

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e_i should be close to

$$\sum_{v_j \in N^{out}(v_i)} \hat{a}(v_i, v_j) e_j = \sum_{j=1}^n \hat{a}(v_i, v_j) e_j.$$

Linear Algebra Algorithms

Local Linear Embedding (LLE):

The goal is then to **minimize** the following optimization function:

$$\Phi(\mathbf{E}) = \|(I - \hat{\mathbf{A}})\mathbf{E}^T\|_F,$$

where $\|\cdot\|_F$ is the **Frobenius norm**, a natural extension of the Euclidean norm to matrices:

$$\|\mathbf{B}\|_F = \sqrt{\sum_{i=1}^m \sum_{j=1}^n b_{i,j}^2}.$$

Linear Algebra Algorithms

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- $\mathbf{E}\mathbf{E}^T/n = \mathbf{I}$, that is, **rows of \mathbf{E} have equal norms** and are **mutually orthogonal**; knowing one of the dimensions of the embedding provides no information about the missing dimensions.

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Result: there is a **unique solution** (up to the rotation).

Linear Algebra Algorithms

Local Linear Embedding (**LLE**):

...

$$\Phi(\mathbf{E}) = \text{tr}(\mathbf{E}(I - \hat{\mathbf{A}})^T(I - \hat{\mathbf{A}})\mathbf{E}^T)$$

Linear Algebra Algorithms

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$\Phi(\mathbf{E})$ is minimized for \mathbf{E} consisting of rows taken as k eigenvectors corresponding to smallest eigenvalues of $(I - \hat{\mathbf{A}})^T(I - \hat{\mathbf{A}})$, excluding the smallest eigenvalue that is equal to 0 (which produces a non-centred eigenvector as discussed above).

Linear Algebra Algorithms

Laplacian Eigenmaps (LEM):

Uses the graph Laplacian matrix $\mathbf{L} = \mathbf{D} - \mathbf{A}$.

This time our goal is to minimize the following optimization function:

$$\Phi(\mathbf{E}) = \sum_{(v_i, v_j) \in V^2} \|e_i - e_j\|^2 a(v_i, v_j) = \text{tr}(\mathbf{E} \mathbf{L} \mathbf{E}^T),$$

that is, points that are connected by heavily weighted edges should be close to each other in the embedded space.

Linear Algebra Algorithms

Laplacian Eigenmaps (LEM):

As before, the problem can be reduced to finding k eigenvectors corresponding to smallest eigenvalues of $\mathbf{D}^{-1/2}\mathbf{L}\mathbf{D}^{-1/2}$, excluding the smallest eigenvalue that is equal to 0 (the 0 eigenvalue always exists and has multiplicity of one, provided the graph is connected).

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Finally, note that in this procedure one can replace \mathbf{A} by any proximity measure \mathbf{S} as long as it is symmetric.

Linear Algebra Algorithms

Another **general approach** is to find a suitable embedding that **minimizes** the following loss function:

$$\Phi(\mathbf{E}) = \|\mathbf{S} - \mathbf{E}^T \mathbf{E}\|_F,$$

where \mathbf{S} is some **proximity measure** matrix. (Keeping the inner product of the embedding vectors of two given nodes as close as possible to the similarity between the nodes in the graph.)

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High Order Proximity preserved **Embedding** (**HOPE**):

Specific algorithm designed for directed graphs.

$$\Phi(\mathbf{E}_s, \mathbf{E}_t) = \|\mathbf{S} - \mathbf{E}_s^T \mathbf{E}_t\|_F,$$

where \mathbf{E}_s and \mathbf{E}_t are the corresponding matrices of the **source** and the **target** embeddings.

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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Uses the model known as **SkipGram**. Consider a context window of size 5 (that is, we take $\ell = 2$) and the sentence:

*“Graph embedding maps **nodes** to vector space”.*

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Uses the model known as **SkipGram**. Consider a context window of size 5 (that is, we take $\ell = 2$) and the sentence:

“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: E_s ("source") and 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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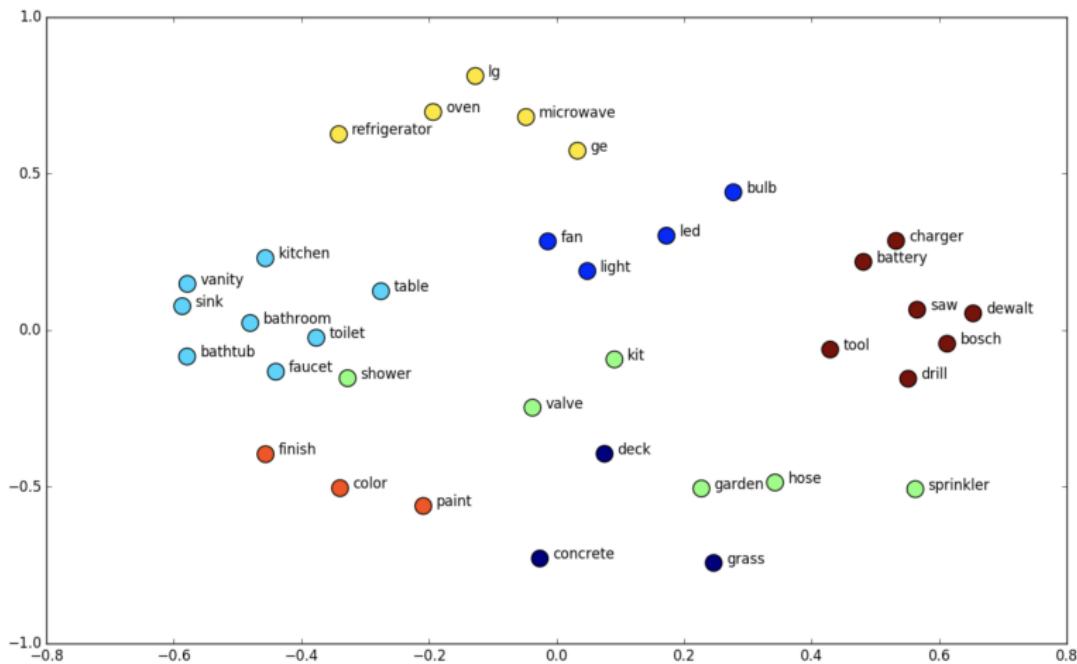
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Given a word i , the probability $p_{i,j}$ that we see word j in its neighbourhood is approximated by the softmax function:

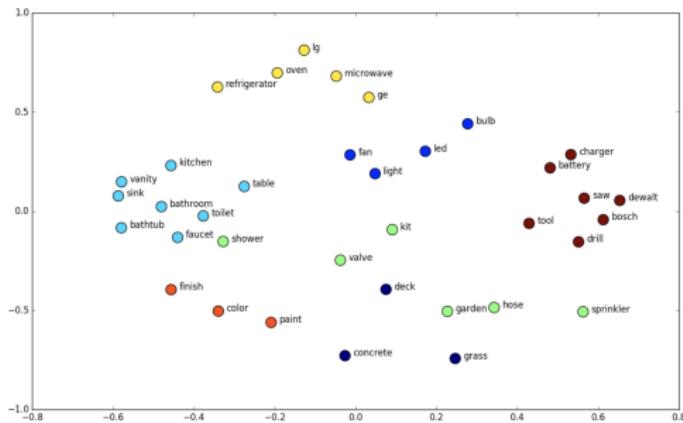
$$q_{i,j} = \frac{\exp(\mathbf{e}_{t,j}^T \mathbf{e}_{s,i})}{\sum_{\ell=1}^{|W|} \exp(\mathbf{e}_{t,\ell}^T \mathbf{e}_{s,i})}.$$

The model is trained using maximum likelihood estimation.

Algorithms Based on Random Walk



Algorithms Based on Random Walk



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

Yet, word embeddings seem to capture these relationships!

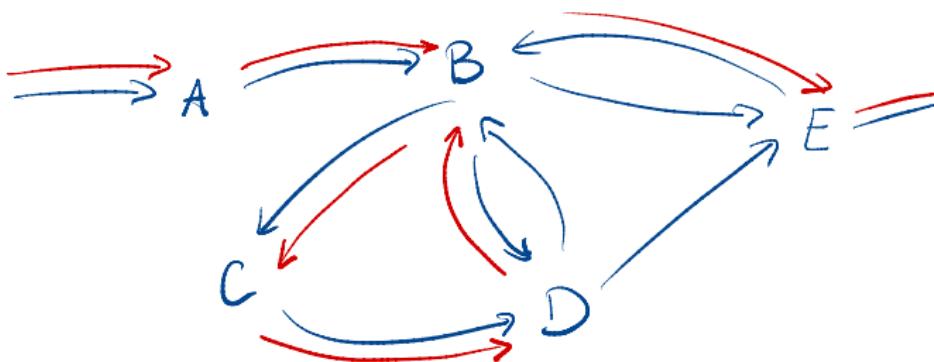
king - man + woman \approx queen

Paris - France + Germany \approx 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).



Walk : ... ABCD BE ...

Algorithms Based on Random Walk

Main challenge: the number of **nodes** is usually **much larger** than the number of **words** in the typical NLP application.
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Solution: use a predictive model called **hierarchical softmax**.
Nodes are represented as leaves in a binary tree (**Huffman tree**);
a binary classifier is fitted at each split. As a result, we only
need to evaluate $\Theta(\ln n)$ classifiers.

Algorithms Based on Random Walk

Deep Walk algorithm:

- Generate **random walks** of some **fixed length**, typically between **32** and **64** per node.

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Deep Walk algorithm:

- Generate **random walks** of some **fixed length**, typically between **32** and **64** per node.
- Depending of the **context window** size, we explore **node's neighbourhoods** beyond the **first** and the **second** order **proximity**.

Algorithms Based on Random Walk

Node2Vec algorithm:

Depending on the parameterization, the random walks are respectively biased toward the following two extremes:

- **Breadth-First Search (BFS)**: walks tend to stay near the initial node and so they mimic the BFS algorithm (they tend to preserve the **macro-view**),
- **Depth-First Search (DFS)**: walks tend to move away from the initial node and so they behave as the DFS algorithm (they tend to preserve the **micro-view**).

The user may smoothly move between these two extremes by changing the parameters of **Node2Vec**, as required in a given application.

Deep Learning Algorithms

Autoencoders:

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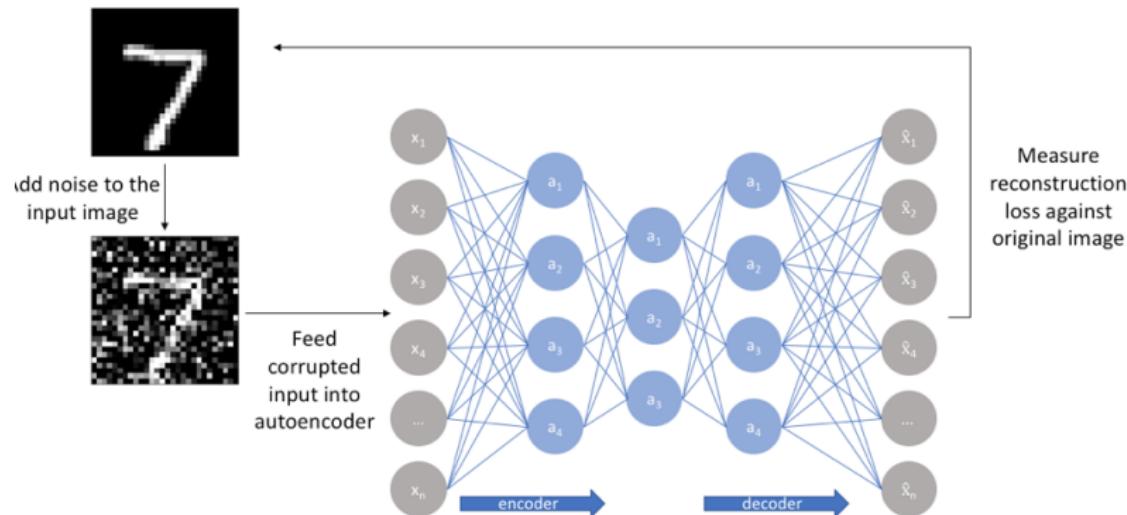
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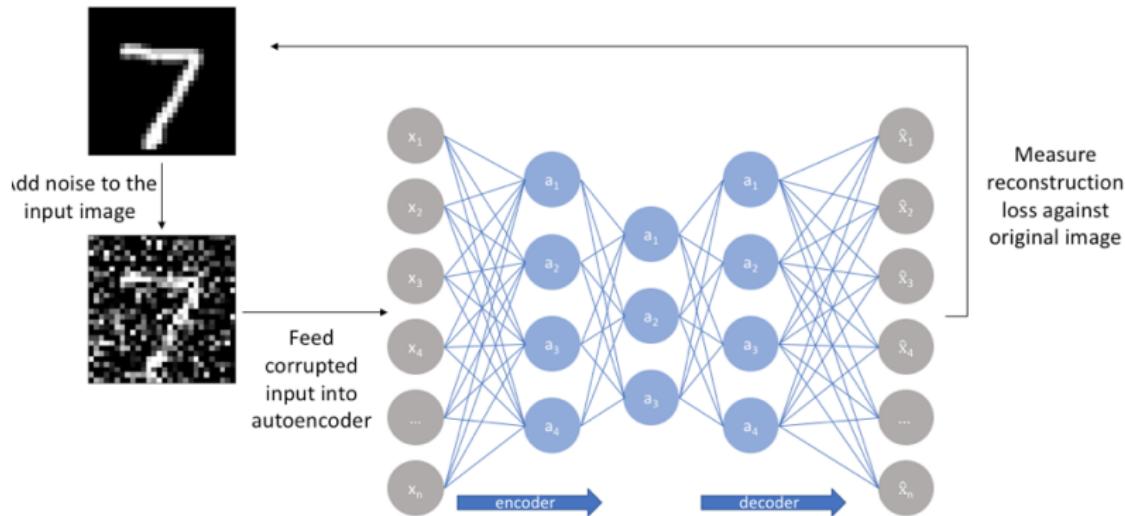
Both functions form the autoencoder that tries to get $D(E(a_i))$ as close to a_i as possible.... well, not only that.

Deep Learning Algorithms



Autoencoders train the network to ignore “noise”.

Deep Learning Algorithms



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Structural Deep Network Embedding (SDNE) is an example of such family of algorithms.

Structural Node Embeddings

Graph Convolution Network (GCN): see the book

Recursive Feature Extraction (ReFeX):

- f_i^0 features associated with node v_i : external metadata or some property of the node such as its degree, clustering coefficient, etc. (f^0 is a vector of vectors.)

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- prune: select a subset I^s of features from
 $\{f^j : j \in \{0, 1, \dots, s\}\}$ that are not redundant.

Structural Node Embeddings

Graph Convolution Network (GCN): see the book

Recursive Feature Extraction (ReFeX):

- f_i^0 features associated with node v_i : external metadata or some property of the node such as its degree, clustering coefficient, etc. (f^0 is a vector of vectors.)

In each step,

- aggregate using some function $a(\cdot)$ (e.g. mean, sum):
$$f_i^s = a(\{f_j^{s-1} : j \in N(v_i)\});$$
- prune: select a subset I^s of features from
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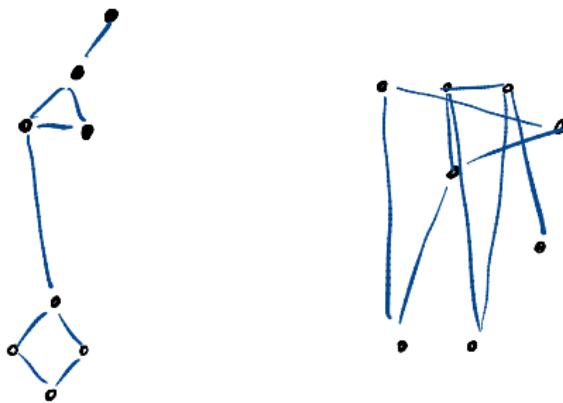
Repeat t times or until no new features are introduced. Vectors from $\bigcup_{j=0}^t I^j$ form the embedding.

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** $\mathbf{w} = (w_1, \dots, w_n)$.

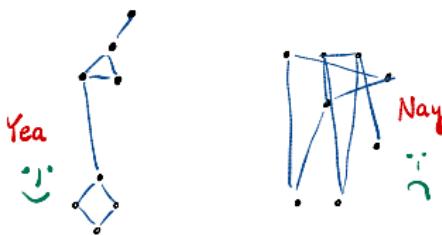
Embedding of nodes of V , $\mathcal{E} : V \rightarrow \mathbb{R}^k$ (typically many).

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Output: two “divergence scores” (**global** and **local**) assigned to \mathcal{E} (smaller is better).



Global Score

Global score:

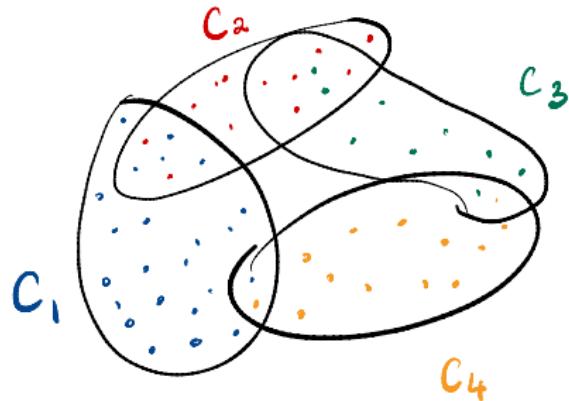
- looks at the network and the associated embeddings “from the distance”;
- evaluates the embeddings based on their ability to capture global properties of the network, namely, edge densities;

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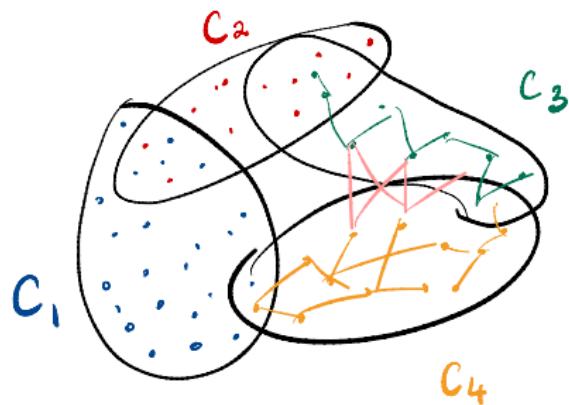
- looks at the network and the associated embeddings “from the distance”;
- evaluates the embeddings based on their ability to capture global properties of the network, namely, edge densities;
- **goodness-of-fit** test for the provided embedding, rather than simply checking its predictive power—its aim is similar to the well-known **Hosmer–Lemeshow** test for logistic regression (used frequently in **risk prediction** models).

Global Score



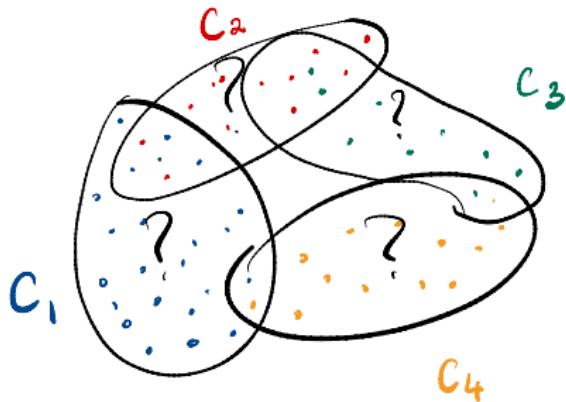
Step 1: Run some graph **clustering** algorithm to obtain a **partition** of V into ℓ communities C_1, \dots, C_ℓ .

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 \mathcal{E} .

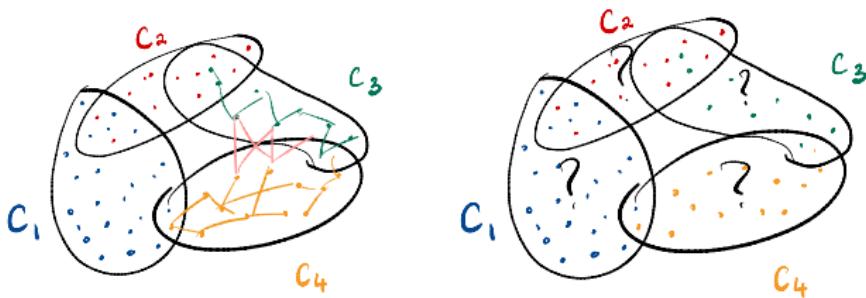
Global Score



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** $\mathcal{G}(\mathbf{w}, \mathcal{E}, \alpha)$.

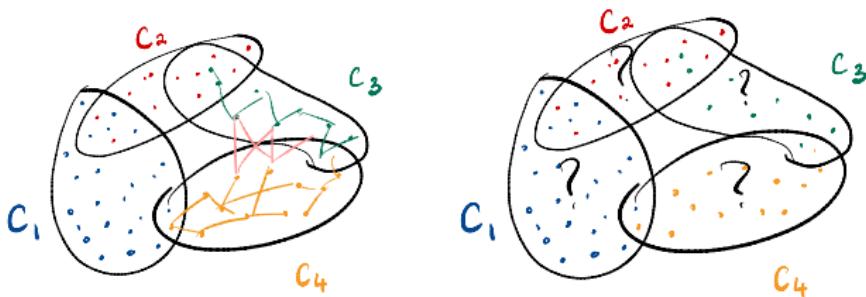
Note that we do **not** use G , only \mathbf{w} (on top of \mathcal{E} and parameter α , the “**aversion**” for **long** links).

Global Score



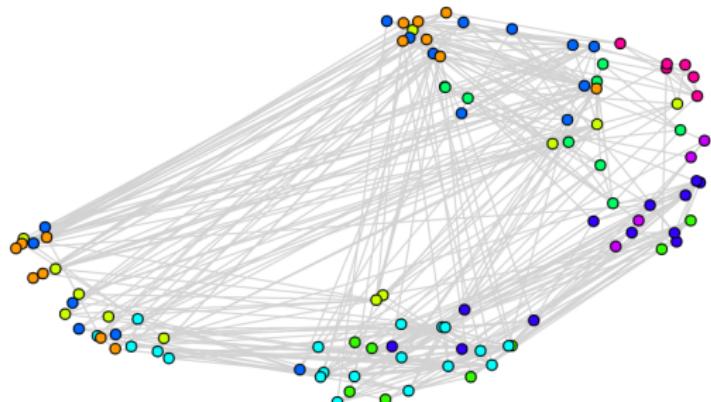
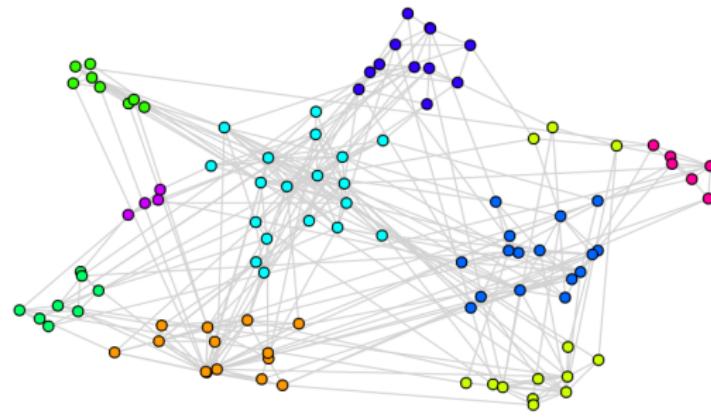
Step 4: Compute Δ_α : the **Jensen-Shannon divergence** between the two vectors (smoothed version of the **Kullback-Leibler** divergence we mentioned earlier).

Global Score

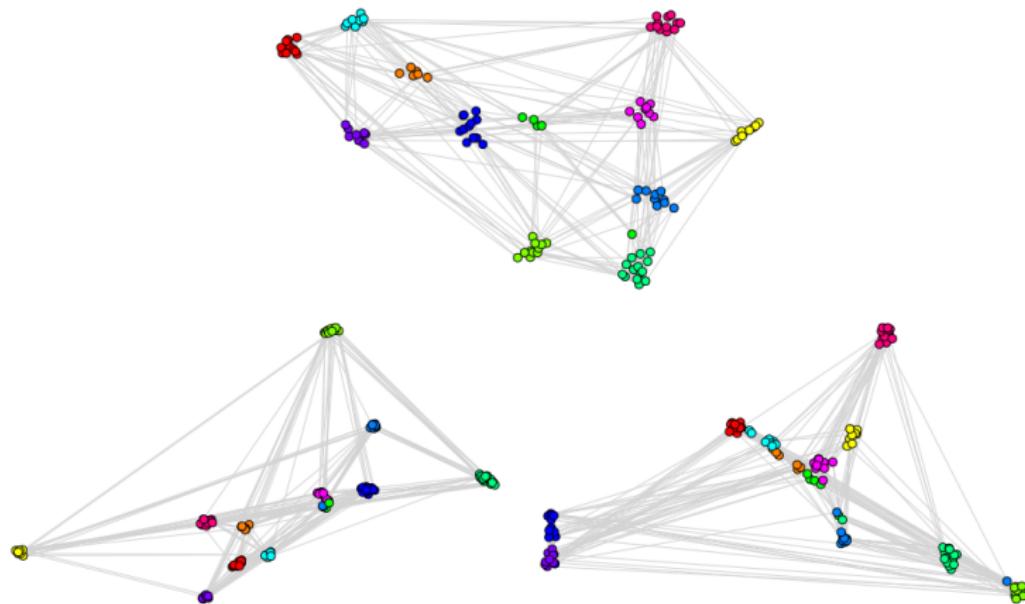


Step 5: Take the minimum Δ_α over various choices for parameter α that measures the “aversion” for **long** links.
It defines the **global** score.

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.

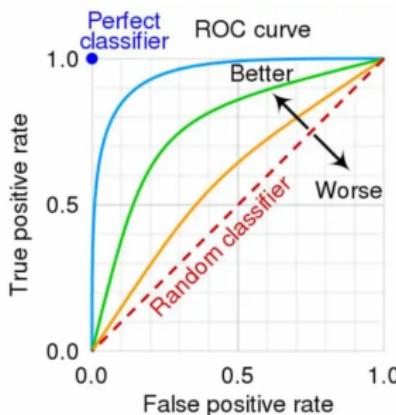
Local Score

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.
- 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



Local Score

- The **AUC** (area under the ROC curve) provides an aggregate measure of performance across all possible classification thresholds which can be interpreted as the probability that a randomly chosen positive sample is ranked higher than a negative sample:

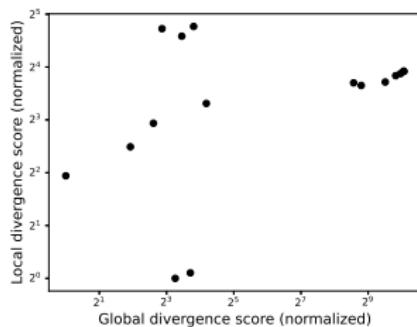
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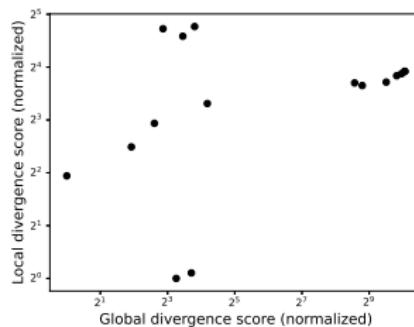
$$\frac{\sum_{st \in S^+} \sum_{uv \in S^-} \mathbf{1}\{p(s, t) > p(u, v)\}}{|S^+| \cdot |S^-|}.$$

(Can be easily approximated by **sampling**.)

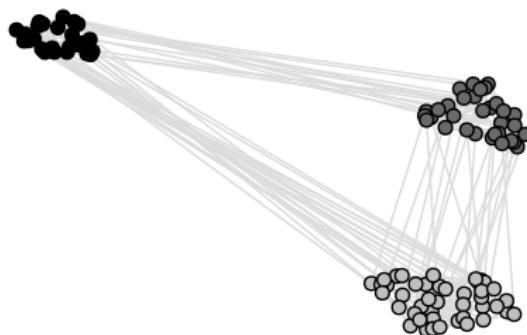
Example: ABCD (3 communities)



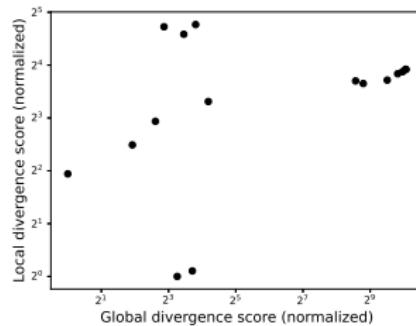
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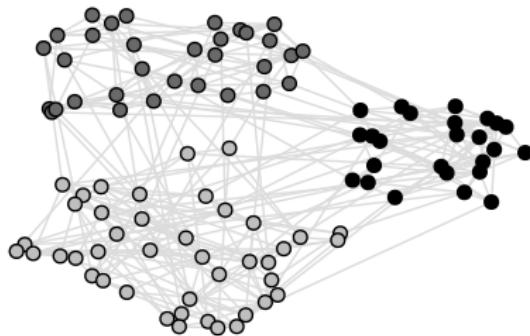
Low global divergence



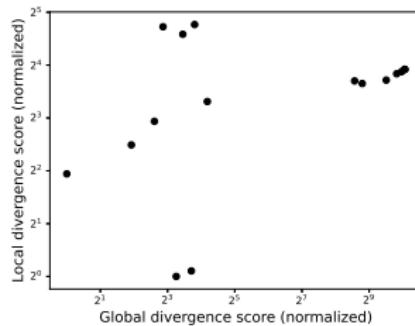
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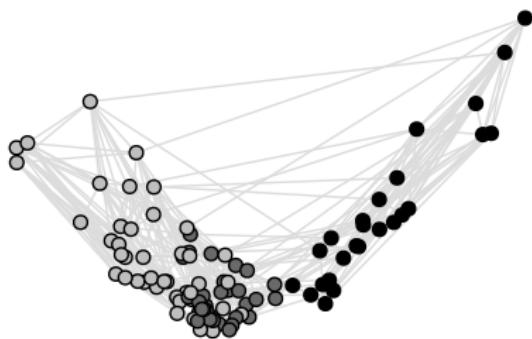
Low local divergence



Example: ABCD (3 communities)



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 $d_{i,j} = \text{dist}(\mathcal{E}(v_i), \mathcal{E}(v_j))$ 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 \mathcal{E} .

Geometric Chung-Lu model

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

This part requires $\Theta(n^2)$ steps and so it is not feasible for large graphs.

Geometric Chung-Lu model

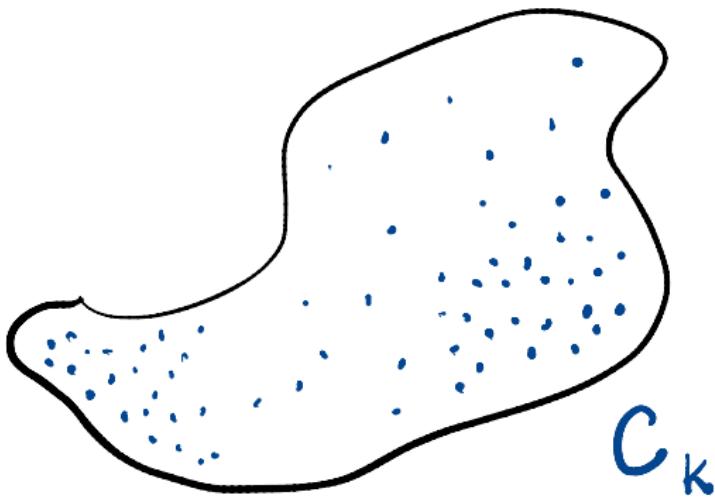
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We propose **scalable** (approximation) algorithm with running time $O(n \ln n)$.

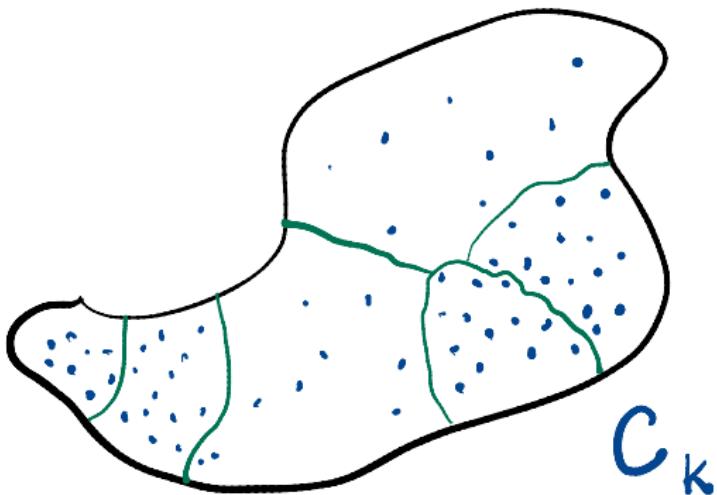
Scalable Algorithm — Main Idea

Independently consider each part.



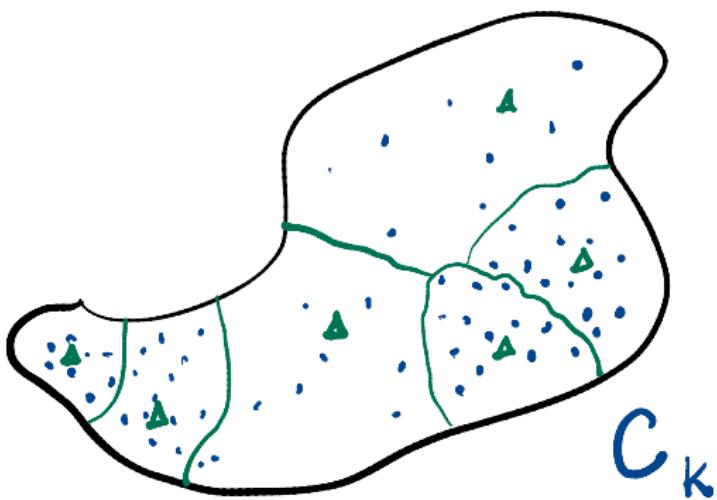
Scalable Algorithm — Main Idea

Group together nodes that are close to each other in the embedded space.



Scalable Algorithm — Main Idea

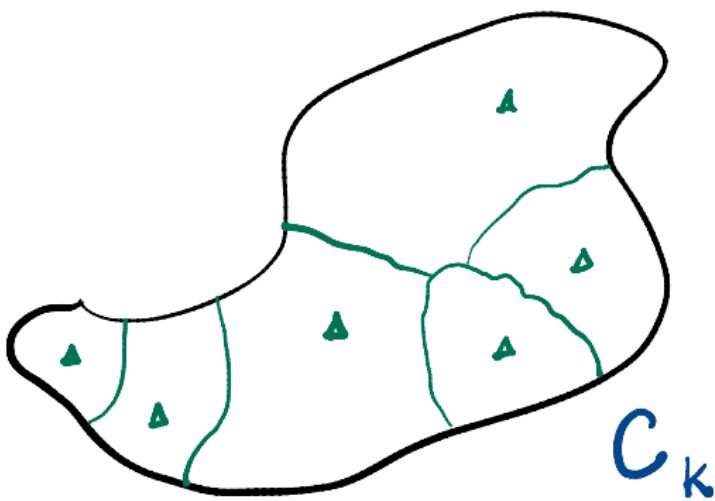
Replace each group by the corresponding auxiliary node (**landmark**) that is placed in the (appropriately weighted) **center of mass**.



Scalable Algorithm — Main Idea

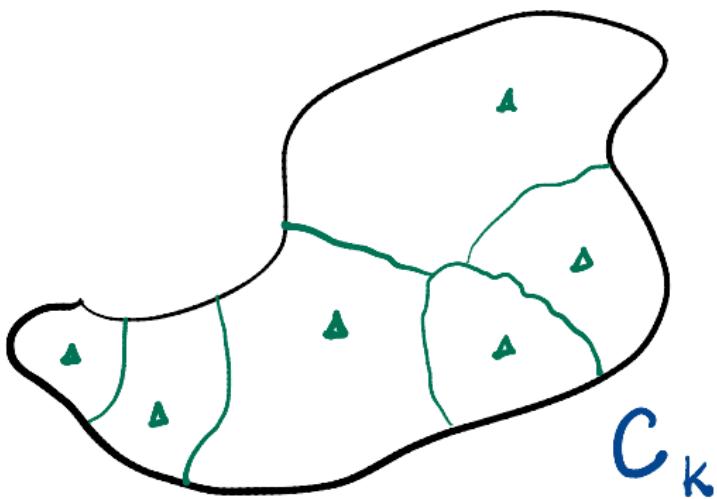
We get **auxiliary graph** with **auxiliary embedding**.

Approximate original $b_{i,j}$ by $a_{i,j}$ obtained for **landmarks**.



Scalable Algorithm — Main Idea

If the number of **landmarks** is $n' \approx \sqrt{n \ln n}$, then tuning weights takes $O((n')^2) = O(n \ln n)$.



Scalable Algorithm — Refining the partition

For each part we compute the **weighted center of mass** p_i and the **weighted sum of squared errors (SSE)**, a natural measure of variation within a part) e_i :

$$p_i := \frac{\sum_{j \in C_i} w_j \mathcal{E}(v_j)}{\sum_{j \in C_i} w_j} \quad \text{and} \quad e_i := \sum_{j \in C_i} w_j \operatorname{dist}(p_i, \mathcal{E}(v_j))^2.$$

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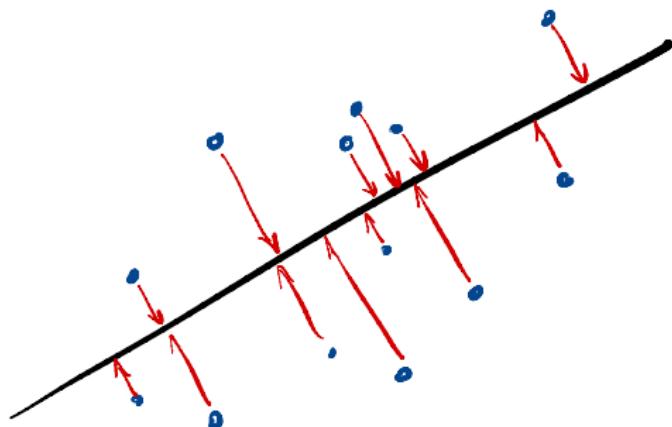
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Split each part **a few times**, and then keep splitting **greedily** (parts with the largest SSE).

Would be nice to split a part with SSE equal to e_i into two parts such that $\max\{e_i^1, e_1^2\}$ is **as small as possible**—difficult and **computationally expensive**.

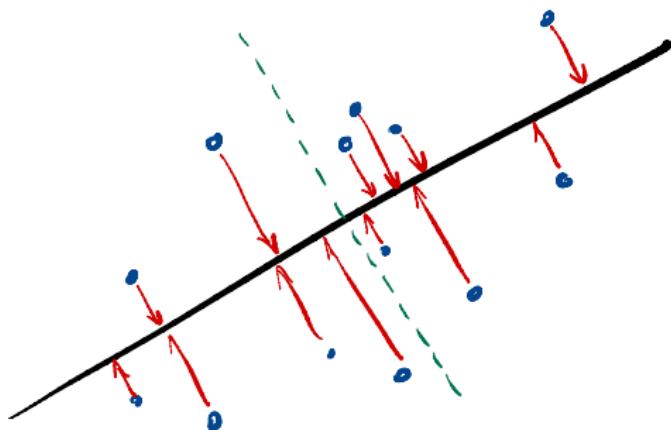
Scalable Algorithm — Refining the partition

Approximate using the well-known **weighted Principal Component Analysis (PCA)** in which the first principal component has the **largest** possible **weighted variance**.



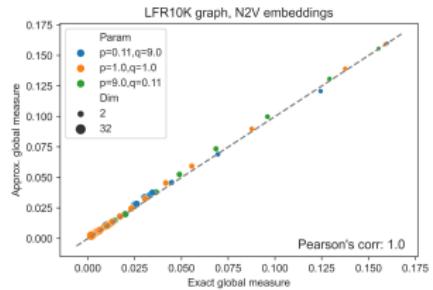
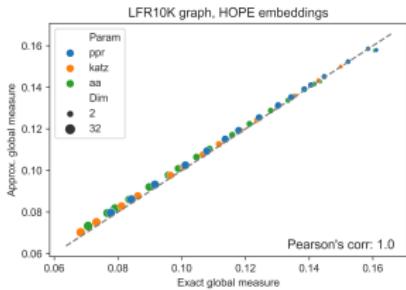
Scalable Algorithm — Refining the partition

We get a **total order** of these points and one can quickly check which of the natural $|C_k| - 1$ partitions minimizes $\max\{e_i^1, e_i^2\}$.



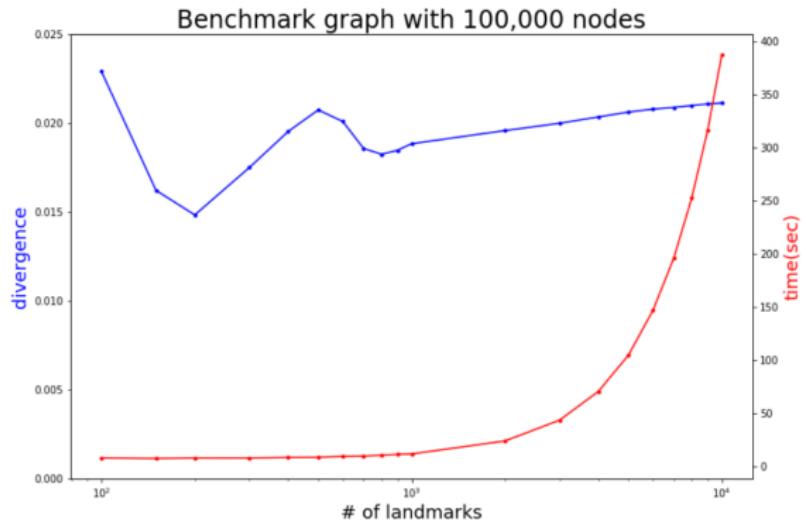
Scalable Algorithm — Quality and Speed Comparison

LFR graph (HOPE and Node2Vec embeddings)



Scalable Algorithm — Quality and Speed Comparison

ABCD graph



We tested n' up to $n' = 10^4 = n^{4/5}$, larger than $n' = \sqrt{n}$.
One can easily deal with graphs of order $n = (10^4)^2 = 10^8$.

A Few Applications

Datasets and Algorithms Used

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- Zachary karate club data set (small, good for visualization),
- synthetic ABCD graph on $n = 1,000$ nodes partitioned into 12 communities (sizes ranging between 50 and 150), $m = 8,327$ edges, and relatively weak community association ($\xi = 0.6$).
- Embedding in 64-dimensional space using HOPE together with Personalized PageRank proximity measure. (It gives good divergence results when using the framework but other choices give similar results).

Node Classification

Embedding algorithms can be viewed as the process of extracting features of the nodes based on the structure of the graph, one may reduce the problem to classical machine learning predictive modeling classification problem for the set of vectors.

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There are many algorithms, such as logistic regression, k -nearest neighbours, decision trees, support vector machine, etc., for any potential scenario that one might be interested in, including binary, multi-class, and multi-label classifications.

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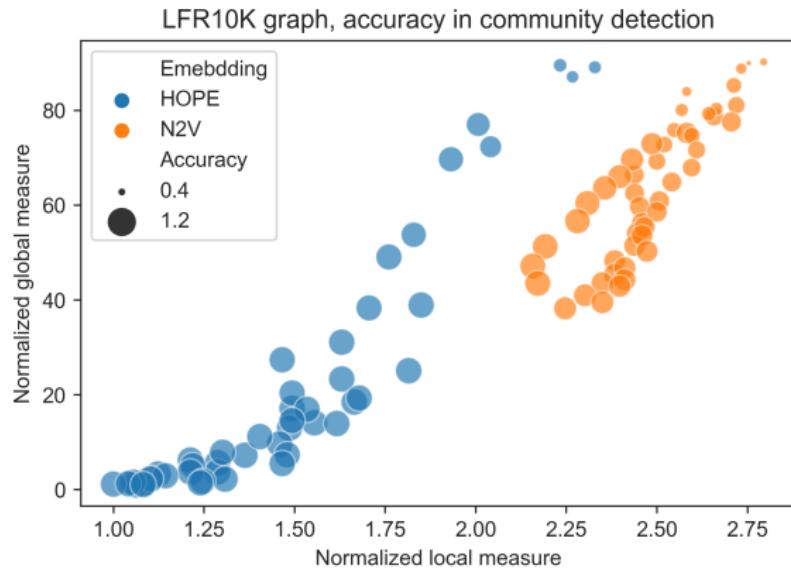
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 - We applied the model to the **test set**. We got **90.9%** overall accuracy which is quite good in comparison to a **random classifier** which gives accuracy under **9%**.

For **multi-class classification**, we often present the **confusion matrix** $\mathbf{C} = (c_{i,j})_{i,j \in [n]}$; $c_{i,j}$ is the **number** of nodes in **community i** classified as being in **community j** . The proportion of **weight** on the **diagonal** is the overall **accuracy** (again, **90.9%**).

$$\mathbf{C} = \begin{bmatrix} 78 & 1 & 4 & 0 & 0 & 2 & 3 & 0 & 3 & 0 & 1 & 0 \\ 0 & 77 & 0 & 1 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 71 & 0 & 1 & 0 & 0 & 0 & 3 & 0 & 0 & 0 \\ 1 & 1 & 1 & 64 & 0 & 1 & 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 2 & 1 & 77 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 54 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 3 & 53 & 3 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 & 0 & 42 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 1 & 45 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 44 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 42 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 4 & 2 & 2 & 1 & 0 & 0 & 35 \end{bmatrix}$$

Node Classification

Correlation between the **global** and **local** scores and the quality of **node classification**.



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One may want to combine the two clustering techniques which presumably should give better results as node embeddings provide some additional information about a function or a role of particular nodes, something that is not available with graph clustering alone.

We try something simple: *k*-Leiden.

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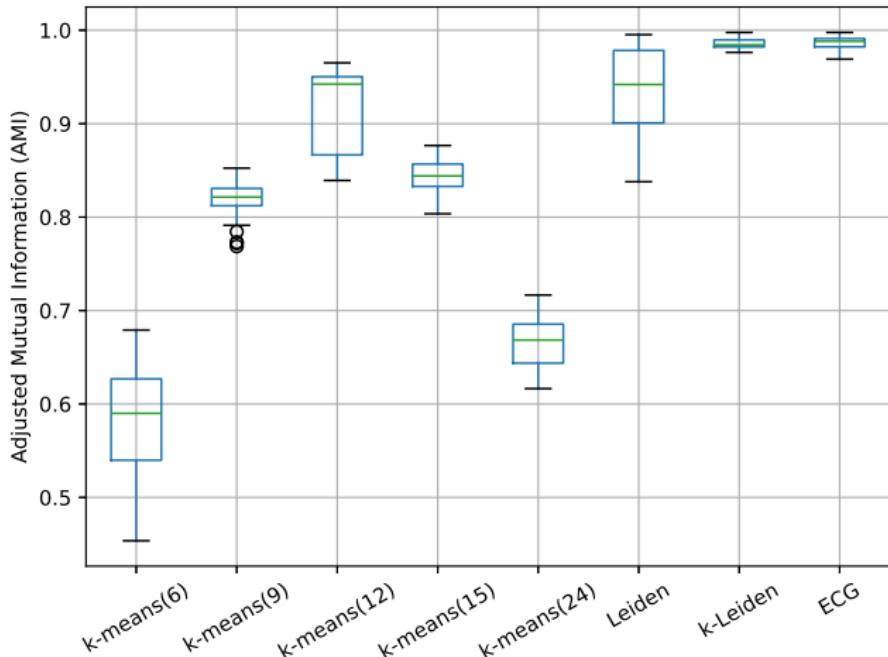
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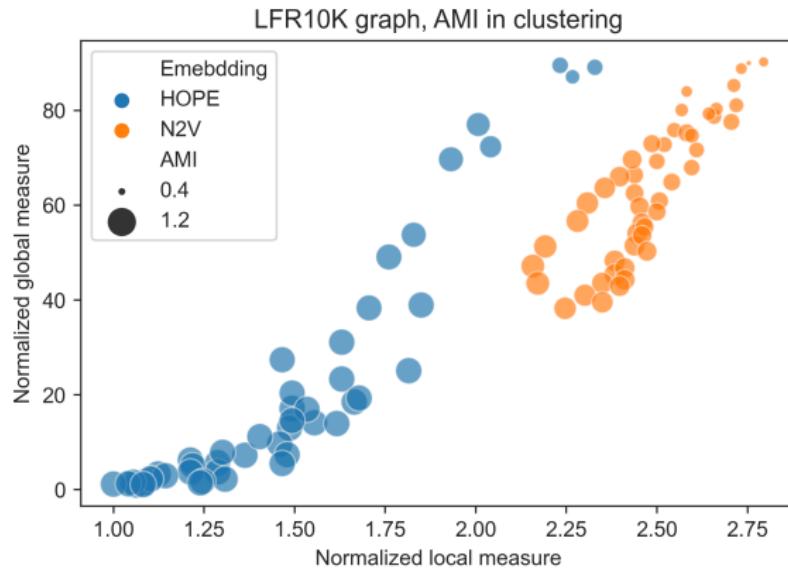
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- For **DB-scan**, since this algorithm is deterministic, we only report that the **AMI** value is equal to **0.67** for all nodes, and **0.88** if outliers are identified by the algorithm and then excluded.

Community Detection



Community Detection

Correlation between the **global** and **local** scores and the quality of **node classification**.



Link Prediction and Missing Links

Node embeddings can also be used to predict:

- missing links (important in biological networks; expensive/difficult/not accurate),
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Link Prediction and Missing Links

Node embeddings can also be used to predict:

- missing links (important in biological networks; expensive/difficult/not accurate),
- links that are likely to be formed in the future (main ingredient of recommender systems).
- Nodes that are close to each other in the embedded space but are not adjacent might get connected in the near future.
- Nodes that are far in the embedded space might get disconnected.

Such behaviour is known in social science as homophily and aversion.

Link Prediction and Missing Links

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- **Remove** randomly **10%** of edges to form G' .

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- We used the **logistic regression model** (using the L_1 -distance between the nodes' embeddings) in which the output is an estimation of the **probability** for the **positive** class in the training data set.

Link Prediction and Missing Links

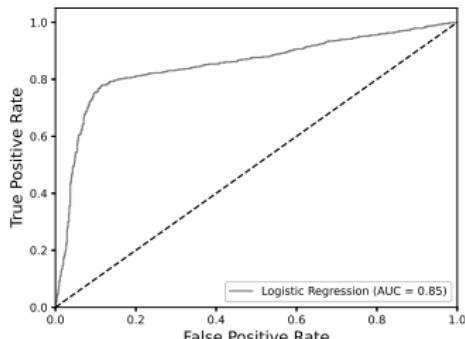
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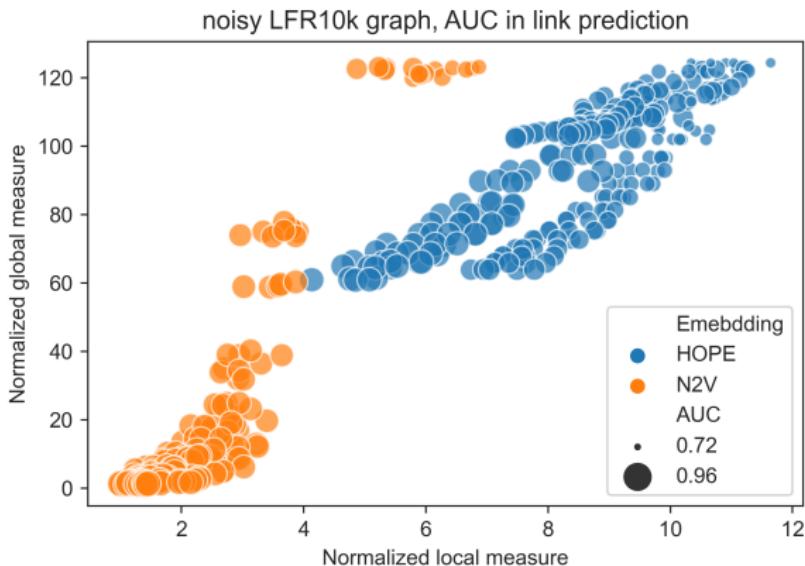
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- We got 61% accuracy for $\xi = 0.6$ and 83% for $\xi = 0.2$ — it works well in comparison to the random classifier that has 50% accuracy.
- The results are usually presented in the form of the Receiver Operating Characteristic curve (ROC curve).



Link Prediction and Missing Links

Correlation between the **global** and **local** scores and the quality of **link prediction**.



Visualization

- There are some **specialized** algorithms (**layouts**).

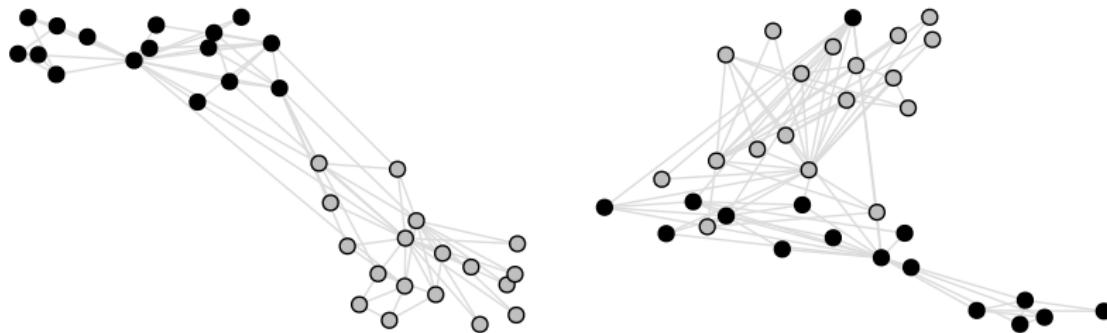
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- There are some **specialized** algorithms (**layouts**).
- Embed G in k -dimensional space (k relatively large).
- Use some generic **dimensionality reduction techniques** to go down to **2D**: Principal Component Analysis (PCA) or t -Distributed Stochastic Neighbour Embedding (t -SNE).

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- Embed G in k -dimensional space (k relatively large).
- Use some generic **dimensionality reduction techniques** to go down to **2D**: Principal Component Analysis (PCA) or t -Distributed Stochastic Neighbour Embedding (t -SNE).
- We personally recommend **Uniform Manifold Approximation and Projection (UMAP)** that is a novel manifold learning technique for dimension reduction.
- We also recommend to test **various embeddings** and various parameters and select the one that scores well in the **benchmark framework**.

Visualization



Other Directions

Signed Graphs: each edge has a **positive** or **negative** sign (friendly or antagonistic interactions). There are some embeddings, such as **Signed Network Embedding (SNE)**, that are crafted to deal with such networks.

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Embedding Edges: represent **edges** as low-dimensional vectors. One can embed the **nodes** of the **line graph** but there are more approaches.

Multi-Layered Graphs: sometimes we have ℓ graphs available with **overlapping** sets of **nodes**. For example, in protein-protein interaction networks derived from different tissues (say, from brain and liver tissues), some proteins occur across multiple tissues.

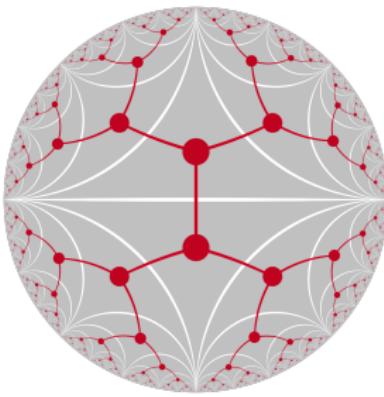
Other Directions

Hyperbolic Spaces: real-world graphs with **scale-free** or **hierarchical** structure might produce outcomes with relatively large distortion (**graph distances** cannot be accurately estimated based on the **Euclidean distances**).

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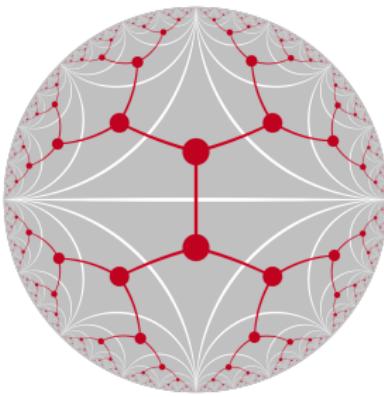
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Hyperbolic Graph Convolutional Neural Network (**HGCN**) is the first inductive hyperbolic counterpart of **GCN**.

Other Directions

Embedding Graphs: map the graph to a point in a vector space.

Two families: **explicit** graph embeddings (return embeddings) and **implicit** ones that are also known as graph kernels (provide a pairwise similarity measure between graphs).

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We experimented with **Graph2Vec** (deep learning) in complementary material.

We used two well-known datasets (**NCI1** and **NCI109**) of **chemical compounds** from the National Cancer Institute screened for activity against non-small cell lung cancer and ovarian cancer cell lines.

Experiments

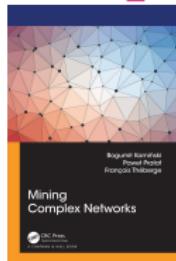
Experiments

Jupyter notebooks and datasets that accompany the textbook/slides are available on GitHub:

<https://github.com/ftheberge/GraphMiningNotebooks>

[Python_Notebooks_Second_Edition](#)

[Julia_Notebooks_2nd](#)



Tutorials for Python notebooks can be found on YouTube:

<https://www.youtube.com/@MiningComplexNetworks>

THE
END