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Systematic comparison of graph embedding methods in practical tasks

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Network embedding techniques aim at representing structural properties of graphs in geometric space. Those representations are considered useful in downstream tasks such as link prediction and clustering. However, the number of graph embedding methods available on the market is large, and practitioners face the non-trivial choice of selecting the proper approach for a given application. The present work attempts to close this gap of knowledge through a systematic comparison of eleven different methods for graph embedding. We consider methods for embedding networks in the hyperbolic and Euclidean metric spaces, as well as non-metric community-based embedding methods. We apply these methods to embed more than one hundred real-world and synthetic networks. Three common downstream tasks — mapping accuracy, greedy routing, and link prediction — are considered to evaluate the quality of the various embedding methods. Our results show that some Euclidean embedding methods excel in greedy routing. As for link prediction, community-based and hyperbolic embedding methods yield overall performance superior than that of Euclidean-spacebased approaches. We compare the running time for different methods and further analyze the impact of different network characteristics such as degree distribution, modularity, and clustering coefficients on the quality of the embedding results. We release our evaluation framework to provide a standardized benchmark for arbitrary embedding methods.

I. INTRODUCTION

Representing complex networks in latent space, or net-10 work embedding, has generated a growing interest from 11 multiple disciplines [1-3]. From a theoretical point of 12 view, the geometric representation of a network may pro-13 vide an intuitive explanation of key properties of real-14 world systems such as structural features [4], navigabil-15 ity [5, 6], and robustness [7, 8]; when it comes to ap-16 plications, network embedding can be useful for graph 17 analysis tasks like visualization [9], link prediction [10], 18 and graph clustering [11, 12]. 19

Many embedding methods use Euclidean space as their 20 ²¹ target space. Euclidean embedding is intuitive and can immediately be used in standard machine learning algo-22 rithms [2, 3]. However, network embedding methods are 23 not limited to Euclidean space. For example, many re-24 cent approaches represent networks in hyperbolic space, 25 where properties like hierarchy and heterogeneity can be 26 easily captured [13–17]. Community structure can be 27 seen as an alternative approach to network embedding in 28 non-metric spaces [18]. 29

The existence of so many available and diverse em-30 bedding techniques presents a challenge for practitioners 31 when they have to choose the proper method for the ap-32 blication at hand. Standardized tests for systematic com-33 parison among methods are lacking. The effectiveness 34 of embedding methods is generally measured on limited 35 types of tasks and small corpora of real-world networks. 36 As a result, gauging the relative performance of a method 37 with respect to another is difficult. 38

³⁹ In this work, we address this gap of knowledge by

40 performing a systematic comparison of representative ⁴¹ embedding methods. We consider five hyperbolic em-⁴² bedding methods (HyperMap [13, 19], Mercator [14], ⁴³ Poincaré maps [15], Hydra [16], and HyperLink [17]), ⁴⁴ four Euclidean-space-based approaches (Node2vec [20], ⁴⁵ Laplacian Eigenmaps (LE) [21], HOPE [22], and ⁴⁶ Isomap [23]), and the two variants (relying on Lou-⁴⁷ vain [24] and Infomap [25]) of the non-metric community ⁴⁸ embedding method [18]. We apply these methods to em-⁴⁹ bed more than one hundred real-world and synthetic net-⁵⁰ works. Three downstream tasks, i.e., mapping accuracy, ⁵¹ greedy routing, and link prediction, are considered to ⁵² evaluate the quality of the various embedding methods. ⁵³ We assess how the performance of the various methods ⁵⁴ is affected by network characteristics such as degree dis-⁵⁵ tribution, modularity, and average clustering coefficient. The various methods are also compared in terms of their 57 computational complexity and their number of tunable 58 parameters.

Our findings indicate that Euclidean embedding metho ods such as Node2vec and Isomap represent the overall best choice for practitioners as they yield decent performance in all tasks. Hyperbolic embedding methods excel in link prediction; however, their high computational complexity impedes their application to large-scale networks. Community-based methods behave similarly to hyperbolic embedding methods, but they have a lower computational demand. Our systematic analysis includes many different embedding methods. However for obvious reasons, we could not include all methods that are curro rently available on the market or that will be developed in the future. For example, we did not consider geometat https://github.com/yijiaozhang/hypercompare. ¹³¹ in Node2vec embedding.

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GRAPH VISUALIZATION TT

To qualitatively illustrate differences between different 78 network embedding methods, we display graphical visu-¹³⁴ 79 80 network topology, i.e., the autonomous system (AS) In-81 ternet network [30]. The network contains N = 23,74882 nodes and E = 58,414 edges. Visualizations are dis-83 played in Fig. 1. 84

It is important to stress that all visualizations are dis-85 played in the two-dimensional Euclidean space, thus the 86 original embedding is projected in this space using some 87 ad-hoc recipes. For example, to yield decent embed-88 ding results, a high embedding dimension is required 89 for Node2vec, LE, and HOPE. We therefore first learn 90 their 128-dimensional embeddings and then use princi-91 pal component analysis (PCA) to project the results into 92 the two-dimensional plane of the figure. The visualiza-93 94 bedding dimension to two. For hyperbolic embedding ¹⁵⁰ overall performance. 95 methods, we represent the embedded nodes with their po-96 97 the two-dimensional Euclidean projection of the Poincaré 98 disks. Finally, despite their potential use in graph draw-99 100 ing, we exclude the non-metric community-based embed- 155 parameter values for all networks, see Sec. VIIA for de-¹⁰¹ ding methods from the qualitative analysis in order to ¹⁵⁶ tails. avoid the use of sophisticated projections in the two-102 dimensional Euclidean space. 103

To help the readers making sense of the visualizations, 104 we color the autonomous systems, i.e., the nodes of the 105 ¹⁰⁶ network, according to the continents where they are lo- ¹⁵⁸ 107 108 109 110 i.e., nodes within the same continent are often close one 162 rectly finding the embedding configuration that best pre-¹¹¹ to the other in the visualizations. If we consider polar ¹⁶³ serves pairwise distance or other similarity relationships. 112 113 114 115 116 centrality information [31]. 117

To quantify such connection, we use over a dozen real- 170 Sec. VIIA for details). 118 world networks to empirically estimate the Spearman's 171 119 120 ¹²¹ from the geometric center of different embeddings de-¹⁷³ nodes in the space so that pairwise graph proximity r_{c} and different network centrality measures. r_{r} is preserved in the embedding. We quantify the map-¹²³ The results are shown in Fig. 2. Clearly, the radial coor-¹⁷⁵ ping accuracy of an embedding method in terms of the r_{24} dinates r_c of HyperMap, Mercator, and HyperLink rep- r_{76} Spearman's correlation coefficient ρ between the pairwise $_{125}$ resent the degree of the nodes [13, 14, 17]. r_c in the $_{177}$ shortest path distance in the network and the pairwise ¹²⁶ Isomap, Hydra, and Poincaré maps embeddings is highly ¹⁷⁸ distance in the embedding space. Note that it is infea-

⁷² ric embeddings of networks induced by dynamical pro- ¹²⁷ correlated with closeness centrality [31]. For embeddings $_{12}$ cesses [26–29], see Ref. [1] for more examples. To ease the $_{128}$ obtained by LE and HOPE, r_c is highly correlated with ⁷⁴ analysis of arbitrary embedding methods under our pro-¹²⁹ closeness and eigenvector centrality. However, we do not $_{75}$ posed experimental setting, we made it publicly available $_{130}$ find obvious connection between node centrality and r_c

III. PERFORMANCE IN DOWNSTREAM 132 TASKS 133

We now use downstream tasks to quantify the embedalizations produced by the various methods for the same 135 ding quality of different methods. Specifically, we mea-¹³⁶ sure their performance in mapping accuracy, greedy rout-¹³⁷ ing, and link prediction. These tasks are conducted on 72 ¹³⁸ real-world networks representing social, biological, tech-¹³⁹ nological, transportation, and communication systems. 140 Details of these networks are included in Ref. [39], Sec. 141 I.

To summarize the results from all the networks for 142 143 an embedding method on a task, we produce the com-144 plementary cumulative distribution function (CCDF) of 145 a performance metric and calculate the area under the ¹⁴⁶ CCDF curve (CCDF-AUC) as the overall score. The 147 CCDF-AUC matches the average value of the perfor-148 mance metric over the entire corpus of real-world nettion by Isomap is obtained directly by setting the em- 149 works and higher CCDF-AUC values indicate better

Some embedding methods have free parameters that 151 lar coordinates or Poincaré coordinates and plot them in 152 could affect the measured value of the performance met-¹⁵³ ric. We tune the parameters for each method to find the ¹⁵⁴ optimal value of the overall performance, and use these

A Mapping accuracy

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A general principle respected by all the embedding cated in. We can see that, although different embedding ¹⁵⁹ methods is that proximity in the embedding space is methods yield drastically different visualizations, all of 160 representative for similarity or proximity in the original them can preserve geographic proximity to some extent, ¹⁶¹ graph. Indeed, some embedding methods work by dicoordinates for all the embeddings (using the geomet- 164 For example, Isomap, Poincaré maps, and Hydra aim at ric center as the origin for Euclidean embeddings), it 165 preserving the shortest path distance among all pairs of becomes clear that the angular coordinates encode the 166 nodes in the embedding space; Node2vec and HOPE try community structure of the graph [18, 31]. The radial 167 to encode certain similarity information. Other methods coordinates, on the other hand, often convey network 168 follow the principle implicitly by fitting the observed net-¹⁶⁹ work against proximity-preserving network models (see

A natural way to assess the quality of a method is correlation coefficients between the distance of a node 172 to measure how accurately the embedding method maps



FIG. 1. Geometric embedding of the Internet. We display the visualization of the autonomous system (AS) Internet network in Euclidean space inferred by (a) Node2vec, (b) HOPE, (c) LE, (d) Isomap, and in the Euclidean projection of the hyperbolic embedding as inferred by (e) HyperMap, (f) Mercator, (g) HyperLink, (h) Poincaré maps, (i) Hydra. The color of a point is representative for the continent where the corresponding AS is located in. For clarity of the visualization, only nodes with degree larger than one are shown. For the visualization of Node2vec, HOPE, and LE, we first get the coordinates with dimension d = 128, and then use PCA to obtain a two-dimensional projection. For the other methods, we directly plot their two-dimensional embeddings.

TABLE I. Key features and results of different network embedding methods. From left to right, we report: name of the method, the target embedding space (space), programming language of the publicly available implementation (lang.), network structural information preserved by the method (struct. preserv.), computational complexity (complexity), CCDF-AUC for mapping accuracy (mapp. acc.), CCDF-AUC for greedy routing (greedy rout.), and CCDF-AUC for link prediction (link pred.). For each task, we highlight in **bold** face the CCDF-AUC values of the top three embedding methods. In the expressions of computational complexity, N is the number of the nodes, E is the number of the edges, d is the embedding dimension, C is the cost to compute each entry of the shortest path length matrix, e is the number of epochs (we set e = 1,000), $b = \min\{512, N/10\}$ is the batch size, m is the number of node layers, and $\langle k \rangle$ is the average degree of the network. More details about the methods can be found in Sec. VIIA. The CCDF-AUC values are generated by aggregating the performance on 72 real-world networks for mapping accuracy and greedy routing. For link prediction, the CCDF-AUC values are computed on a subset of 46 real-world networks with size larger than 300. The CCDF-AUC values for HyperLink are marked with * because the method is unable to embed several networks. Restricting the analysis on the subset of real-world networks that HyperLink can process yields qualitatively similar results in all three tasks (see Ref. [39], Sec. II).

Method	Space	Lang.	Struct. preserv.	Complexity	Mapp. acc.	Greedy rout.	Link pred.
Node2vec [20]	Euclidean	Python	Tunable	O(dN)	0.561	0.818	0.787
HOPE [22]	Euclidean	Python	Global	$O(d^2 E)$	0.575	0.703	0.769
Laplacian Eigenmaps (LE) [21]	Euclidean	Python	Local	$O(d^2 E)$	0.464	0.566	0.749
Isomap [23]	Euclidean	Python	Global	$O(CN^2 + dN^2)$	0.858	0.861	0.848
HyperMap [19]	hyperbolic	C++	Local	$O(N^2)$	0.388	0.584	0.840
Mercator [14]	hyperbolic	Python	Local	$O(N^2)$	0.557	0.530	0.902
HyperLink [17]	hyperbolic	C++	Local	$O(m\langle k\rangle N^2)$	0.516*	0.510*	0.897^{*}
Poincaré maps [15]	hyperbolic	Python	Global	$O(N^2 + ebN)$	0.628	0.494	0.822
Hydra [16]	hyperbolic	R	Global	$O(N^{\alpha}), \alpha > 2$	0.799	0.683	0.846
Community embedding (Infomap) [18]	non-metric	Python	Local	$O(N \log N)$	0.618	0.619	0.902
Community embedding (Louvain) [18]	non-metric	Python	Local	$O(N \log N)$	0.561	0.454	0.914

179 sible to consider every possible pair of nodes for large 186 CCDF for some selected methods only. The CCDF-AUC ¹⁸⁰ networks. We therefore use a maximum of 10⁵ random ¹⁸⁷ values of all embedding methods are listed in Table I. $_{181}$ pairs of nodes to approximate the Spearman's ρ in case $_{188}$ Overall, we find that all methods do a good job in prethe total number of node pairs $N(N-1)/2 > 10^5$. 182

¹⁸⁹ serving graph proximity in the embedding space.

183 ¹⁸⁴ racy of different embedding methods on 72 real-world ¹⁹¹ finding is not surprising given that both methods aim

As mentioned above, we calculate the mapping accu-¹⁹⁰ Isomap and Hydra top the ranking on this task. The 185 networks. For sake of clarity, in Fig. 3(a), we plot the 192 at optimizing the congruence between pairwise proxim-



Interpretation of the radial coordinates in FIG. 2. embedding space. We show the pairwise Spearman's correlation coefficients between the distance of a node from the geometric center of different embeddings and different centrality metrics such as closeness[32], eigenvector[33], adaptive degree[34], betweenness[35], PageRank[36], Katz[37], degree, and K-core[38] centralities. The values are obtained by averaging the results from 13 real-world networks with size $N \in [1000, 5000]$ in our dataset.

¹⁹³ ity of nodes in the graph and in the embedding space. The mapping accuracy of Poincaré maps is not as high even though it also aims at preserving the shortest dis-195 tance among pairs of nodes. An advantage of Isomap and 196 Hydra is that they can perform embedding in arbitrarily 197 high-dimensional spaces, while Poincaré maps can only 198 work in two-dimensional hyperbolic space. Our experi-199 ments show that the mapping accuracy of Isomap and 200 Hydra increases as the embedding dimension increases. 201 The results of Fig. 3(a) and Table I are obtained with 202 d = 128. By setting d = 2, Poincaré maps achieves the best performance; the performance of Hydra is also better 204 than that of Isomap. The main reason is that the two-205 dimensional Euclidean space may not be large enough to ²⁰⁷ properly embed large networks (see Ref. [39], Sec. II).

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в. Greedy routing

Network embeddings may be used in greedy routing 209 ²¹⁰ protocols devised for efficient network navigation [5, 74]. The task regards the delivery of a packet from a source 211 node s to a target node t. The packet performs hops on 212 the network edges, moving from one node to one of its 213 neighbors at each stage of the navigation process. In par-214 ticular, according to the greedy protocol, at every stage of the process the packet moves to the neighbor that is 216 $_{217}$ closest to target t according to a metric of distance. Such ²¹⁸ a metric of distance is computed using knowledge about ²⁶⁸ ²¹⁹ the embedding space and the nodes' coordinates. If the ²⁶⁹ formance of graph embedding methods [3, 10]. The goal

 $_{220}$ packet reaches the target node t, the delivery is consid-²²¹ ered successful. However, if the packet visits the same ²²² node twice, the delivery fails. A good embedding for this 223 task should be able to allow a high rate of successful 224 deliveries along delivery paths that are not much longer ²²⁵ than the true shortest paths.

In this work, we follow the literature and use the greedy ²²⁷ routing score (GR score) to measure the performance of ²²⁸ different embeddings in greedy routing [75]. The GR ²²⁹ score is defined as

$$GR \text{ score} = \frac{2}{N(N-1)} \sum_{i>j} \frac{D_{ij}}{R_{ij}}, \qquad (1)$$

 $_{230}$ where D_{ij} is the shortest path length between nodes i ²³¹ and j in the original network, and R_{ij} is the length of ²³² the actual delivery path followed by the packet accord-233 ing to the greedy routing protocol. All pairs of nodes are $_{234}$ considered in the sum of Eq. (1), including those leading 235 to successful and unsuccessful deliveries. For an unsuc-²³⁶ cessful delivery, R_{ij} is infinite and $D_{ij}/R_{ij} = 0$. For a 237 successful delivery along one of the shortest paths con-²³⁸ necting *i* to *j*, we have $D_{ij}/R_{ij} = 1$. The GR score is 0 ²³⁹ when all the deliveries are unsuccessful. The GR score ²⁴⁰ equals 1 when all packets are successfully delivered along ²⁴¹ the shortest path in the original network. Note that it ²⁴² is impossible to test every pair of source-target nodes for ²⁴³ large networks. In our experiments, we randomly select $_{244}$ 10⁴ source-target pairs to approximate the GR score in ²⁴⁵ case the total number of node pairs $N(N-1)/2 > 10^4$.

We show the CCDF of the GR scores for selected em-246 ²⁴⁷ bedding methods in Fig. 3(b) and the CCDF-AUC values 248 for all methods in Table I. We note that all methods can 249 facilitate network navigation to some extent. In general, 250 there is a non-trivial relationship between the perfor-²⁵¹ mance in mapping accuracy and the one in greedy rout-²⁵² ing. It is already known that Isomap performs well in this ²⁵³ task [31]. The relatively good performance of Node2vec is ²⁵⁴ instead a new result. In part, the result can be explained ²⁵⁵ by considering that embeddings obtained by Node2vec ²⁵⁶ are based on the exploration of graph paths, a process ²⁵⁷ that well informs a greedy navigation protocol. On the ²⁵⁸ other hand, it seems that Euclidean-space-based embed-²⁵⁹ dings better suit for this task than embedding methods ²⁶⁰ relying on hyperbolic geometry and non-metric spaces. ²⁶¹ A possible explanation of our finding is that many of the 262 non-Euclidean embedding methods focus on preserving ²⁶³ local network properties rather than global ones. The ²⁶⁴ only exception to this rule is Hydra, which in fact dis-²⁶⁵ plays relatively higher performance than that of the other ²⁶⁶ hyperbolic embedding methods.

Link prediction С.

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Link prediction is a standard task to evaluate the per-



Aggregate performance in downstream tasks. We show the complementary cumulative distribution function FIG. 3. (CCDF) of (a) the Spearman's correlation coefficients of the mapping accuracy, (b) the GR scores of greedy routing, and (c) the ROC-AUC scores of link prediction for different embedding methods on real-world networks. The average performance over all networks of an embedding on a task is equal to the area under the curve of the corresponding CCDF. Since most of the embedding methods are stochastic, the data points in the figure are obtained by averaging the results from five independent repetitions.

271 272 case, we first remove 30% randomly chosen edges from 309 Sec. II). 273 the original network while ensuring that the remaining 274 graph is still formed by a single connected component. 275 The removed edges are used as the positive test set. 276 Then, we randomly sample a negative test set of non-277 existent edges with size identical to that of the positive 278 test set. The remaining network is fed to the embedding 279 methods. For each pair of nodes, the closer they are in 280 the embedding space, the more likely they are connected. 281 282 We stress that the information about removed edges is not provided to any embedding methods except for Hy-283 perlink, for which the percentage of the removed edges is 284 an input parameter. 285

286 287 area under the receiver-operating characteristic curve 321 parameters used). 288 (ROC-AUC). The ROC-AUC score ranges from 0.5 to 322 289 1. 290 291 292 293 294 295 296 297 298 299 this task. Mercator and the community-based methods 333 prediction. 300 vield slightly better performance than the other methods. 334 301 302 303 ³⁰⁴ laws for network connections, which immediately provide ³³⁷ network models and the corresponding network charac-³⁰⁵ predictions for missing links. We also measure the area ³³⁸ teristics analyzed in this paper are listed in Table III.

270 is predicting the existence or the non existence of edges 306 under the precision-recall curve (AUPR) for each method between non-observed pairs of nodes. There are poten- 307 in the link prediction task, the results are qualitatively tially many different ways to implement the task. In our 308 similar to those obtained for ROC-AUC (see Ref. [39],

³¹⁰ D. Embedding performance on synthetic networks

In order to systematically analyze the performance 312 of the different embedding methods, we also use 313 34 instances of synthetic networks generated by five 314 types of network models: the popularity-similarity-315 optimization (PSO) model [4, 19], the Lancichinetti-³¹⁶ Fortunato-Radicchi (LFR) model [76], the configuration 317 model with power-law degree distribution and Poisson 318 degree distribution (power-law networks and Poisson net-The ability of an embedding to distinguish the edges 319 works), and the model for spatial networks by Daqing et from the positive and negative sets is measured by the 320 al. [77] (see Sec. VIIB for details of network models and

We apply the embedding methods to the synthetic For perfect prediction, the ROC-AUC score equals ³²³ networks, repeat the evaluation on three downstream to 1. The score is 0.5 for random guesses. For small ³²⁴ tasks and report the performance in Table II. We can networks, removing 30% of the edges may substantially 325 see that the results on the synthetic network models are distort the network structure and the link prediction re- 326 consistent with the results obtained on the real-world sults. Therefore, we only consider real-world networks ³²⁷ networks. Isomap and Hydra are the top two methwith more than 300 nodes for the link prediction task in 328 ods for mapping accuracy. Euclidean embeddings such this paper. We show the CCDF of ROC-AUC scores for 329 as Node2vec and Isomap perform better than hyperselected embedding methods in Fig. 3(c) and report the 330 bolic and community-based embeddings on greedy rout-CCDF-AUC values for all methods in Table I as before. 331 ing, while hyperbolic and community-based embeddings All embedding methods yield comparable performance in 332 outperform Euclidean-based embedding methods on link

By tuning the parameters of the network models, we The result can be a reflection of the fact that the embed-³³⁵ can further study the effect of network characteristics on dings are obtained by fitting graphs against probability 336 the performance of different embedding methods. The

TABLE II. Embedding performance on synthetic networks. We summarize all the results obtained by the different embedding methods on the synthetic network models considered in this paper (i.e., PSO models, LFR networks, power-law networks, spatial networks, and Poisson networks). From left to right, we report: name of the method, the CCDF-AUC of mapping accuracy on the various network models, the CCDF-AUC of greedy routing scores on the same set of network models, and the CCDF-AUC of link prediction ROC-AUC scores on the same set of network models. Link prediction results for Poisson networks are excluded since no meaningful prediction can be made for the edges of random and homogeneous networks. See details about synthetic networks in Sec. VIIB. We highlight in bold face the top three methods for each network model and task combination. Some values for Mercator and HyperLink are marked with * because the methods are not able to embed several networks. The results are qualitatively similar if we restrict the analysis on the subset of networks that all methods can process.

	Mapping accuracy			Greedy routing				Link prediction						
Method	PSO	LFR	power-law	spatial	Poisson	PSO	LFR	power-law	spatial	Poisson	PSO	LFR	power-law	spatial
Node2vec	0.710	0.626	0.692	0.692	0.578	0.892	0.886	0.925	0.903	0.876	0.825	0.674	0.491	0.770
HOPE	0.740	0.444	0.662	0.547	0.442	0.742	0.740	0.873	0.775	0.768	0.750	0.678	0.523	0.697
LE	0.540	0.462	0.523	0.485	0.452	0.785	0.641	0.673	0.662	0.692	0.762	0.662	0.607	0.618
Isomap	0.943	0.789	0.853	0.863	0.652	0.872	0.846	0.887	0.885	0.794	0.818	0.729	0.647	0.733
HyperMap	0.379	0.314	0.365	0.283	0.266	0.797	0.265	0.528	0.371	0.294	0.848	0.695	0.653	0.660
Mercator	0.459^{*}	0.384	0.375	0.450	0.339	0.607^{*}	0.198	0.253	0.298	0.192	0.847^{*}	0.698	0.623	0.687
Poincaré maps	0.618	0.379	0.412	0.489	0.315	0.577	0.256	0.228	0.418	0.218	0.808	0.672	0.590	0.680
HyperLink	0.303	0.375	0.370	0.345	0.317^{*}	0.593	0.295	0.313	0.355	0.233*	0.742	0.719	0.642	0.662
Hydra	0.898	0.666	0.773	0.685	0.528	0.765	0.371	0.574	0.422	0.480	0.783	0.671	0.663	0.632
Comm. (Infomap)	0.586	0.434	0.402	0.437	0.329	0.743	0.318	0.473	0.442	0.360	0.883	0.735	0.633	0.738
Comm. (Louvain)	0.543	0.384	0.353	0.388	0.309	0.592	0.178	0.185	0.203	0.149	0.883	0.740	0.638	0.732

TABLE III. Synthetic network models considered in our analvsis together with the corresponding network characteristics varied in our tests.

Network model	Characteristic
PSO model [4, 19]	Clustering coefficient
LFR model [76]	Modularity
Poisson network	Average degree
power-law network	Power-law exponent
spatial networks [77]	Power-law exponent

We find that certain network characteristics have 339 ³⁴⁰ strong effects on downstream tasks as follows: (1) the ³⁴¹ ability of embedding methods to preserve graph distance deteriorates as the density of the network grows: (2) 342 the ability of embedding methods to inform the greedy 343 routing protocol improves as the network clustering co-344 efficient increases but its modularity decreases; (3) the 345 ability of embedding methods in inferring links between 346 non-observed pairs of nodes improves as the network 347 ³⁴⁸ clustering coefficient increases, the network modularity 349 grows, and the heterogeneity of the degree distribution ³⁵⁰ increases. Detailed results can be found in Ref. [39], Sec. IV. These effects are universal across different meth-351 352 ods with a few exceptions. For example, Isomap and Node2vec perform well in greedy routing regardless of 353 ³⁵⁴ the network characteristics.

Summary of the results Е.

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356 357 358 359 same analysis for synthetic networks can be found in 374 eral rule of thumb, methods that preserve local informa-



FIG. 4. Average performance in link prediction and greedy routing over a large corpus of real-world networks. We summarize here the same results as of Table I. We plot the CCDF-AUC values of ROC-AUC scores and GR scores for different embedding methods. Circles, triangles and squares represent Euclidean-, hyperbolic- and communitybased embedding methods, respectively. The hollow and solid symbols represent methods that preserve local and global network structural information, respectively.

³⁶⁰ Ref. [39], Sec. IV. We can see that Isomap and Node2vec ³⁶¹ outperform the other methods in greedy routing while ³⁶² community embedding, Mercator, and HyperLink yield ³⁶³ better performance in link prediction. However, no single ³⁶⁴ method outperforms all the other methods in both tasks ³⁶⁵ according to Fig. 4.

We remark that the two tasks are fundamentally dif-366 ³⁶⁷ ferent, as link prediction is a local prediction task while ³⁶⁸ greedy routing is a global discovery task. Also, the po-³⁶⁹ sition of an embedding method in the performance dia-³⁷⁰ gram shown in Fig. 4 seems partially predictable based To provide an overview of the performance of differ- 371 on the type of space targeted by the embedding method ent embedding methods, we focus on link prediction and 372 and/or the type of network structural information that greedy routing, and summarize the results in Fig. 4. The 373 the method is able to preserve (see Table I). As a gen-

³⁷⁵ tion excel in link prediction, and algorithms that preserve 376 global structure achieve optimal performance in greedy 377 routing.



FIG. 5. Greedy routing and link prediction results obtained by Node2vec with different walk length on the IPv6 Internet network. We display (a) the relation between GR score and the shortest path length between node pairs involved when using Node2vec with different walk length (l = 10 and l = 100) to guide greedy routing, (b) same as (a), but for ROC-AUC scores in link prediction, (c) the distribution of distance between node pairs involved in greedy routing, and (d) same as (c), but for link prediction. The data points in the figure are obtained by averaging the results of 10 experiments, the error bars indicate one standard deviation from the mean.

To further validate our rule of thumb, we take advan-378 tage of Node2vec. The algorithm acquires structural in-379 formation by means of random walks with restart. The 380 length of the random walks serves as a proxy for the typ-381 ical scale of structural information that is preserved by 382 the embedding. We apply Node2vec with walk length 383 l = 10 and l = 100 on the Ipv6 Internet network [78] 384 ³⁸⁵ and use the resulting embeddings to perform greedy routing and link prediction. Instead of reporting the overall 386 performance, we group the node pairs involved in the 387 tasks by their shortest path distance in the network and 388 then calculate the scores within each group. For l = 10, 389 the GR score decreases quickly as the distance between 403 putational complexity in Table I. Hyperbolic embedding 390 391 392 the source-to-target distance. Performance in link pre-393 394 diction obtained for l = 10 is far better than the one 407 ³⁹⁵ obtained for l = 100. We note that the vast majority of 396 397 dings obtained for l = 10 and l = 100. 398

IV. COMPUTATIONAL COMPLEXITY AND 399 **RUNNING TIME** 400

401 402 the proper embedding method. We summarize the com- 418 metric embedding methods tend to be much faster than



Running time vs. network size. We show FIG. 6. the running time of different embedding methods in relation to the size of PSO models. The network size ranges from $N = 2^6$ to $N = 2^{15}$. Other parameters of the PSO models are: average degree $\langle k \rangle = 5$, power-law exponent $\gamma = 2.1$, temperature T = 0.5. Each data point is the average of five simulations. For HyperMap, we use the hybrid algorithm without correction steps and enable the speedup mode by setting $k_{\text{speedup}} = 10$ (see Sec. VIIA for details). The black full line indicates linear scaling; the black dashed line denotes quadratic scaling.

TABLE IV. Node2vec and community embedding on large networks. We report the performance on mapping accuracy (Spearman's ρ), greedy routing (GR score), and link prediction (ROC-AUC score) as well as the running time (seconds) of Node2vec and community embeddings with Infomap and Louvain algorithms on the YouTube friend network (N =1,134,890) and the AS Skitter network (N = 1,694,616).

Network	Metric	Node2vec	Infomap	Louvain
YouTube friend	Mapping accuracy	0.620	0.499	0.352
	Greedy routing	0.478	0.071	0.588
	Link prediction	0.959	0.962	0.976
	Running time	$33,045 \ s$	$4,938 \ s$	732 s
AS Skitter	Mapping accuracy	0.582	0.403	0.033
	Greedy routing	0.348	0.117	0.363
	Link prediction	0.998	0.991	0.983
	Running time	$85{,}356~{\rm s}$	$_{3,149~\rm s}$	$1{,}895~{\rm s}$

source and target nodes increases. The performance for $_{404}$ methods have $O(N^2)$ computational complexity at least, l = 100 in greedy routing is instead almost unaffected by $_{405}$ while Euclidean and non-metric methods often scale lin-406 early with the system size.

To directly compare the running time of the various 408 embedding techniques, we apply all the methods to a links tested have distance D = 2, which corresponds to 409 series of networks with different sizes generated by the the maximum gap in performance between the embed- 410 popularity-similarity-optimization (PSO) model [4, 19]. 411 All the experiments are performed on a server equipped 412 with Intel Xeon Platinum 8268 CPUs (2.90GHz) and ⁴¹³ 1.5TB RAM. Although the server have multiple proces-⁴¹⁴ sors, all the methods are allowed to use one processor ⁴¹⁵ only. Figure 6 shows the relation between the running 416 time and the network size for all the embedding meth-Scalability is another important factor when choosing 417 ods. The results confirm that the Euclidean and the non421 tively similar. 422

423 424 munity embedding methods (both variants with Lou- 479 to access and configure, and the method can process dif-425 ⁴²⁶ networks. As a demonstration, we apply them to two ⁴⁸¹ some embedding methods from our experiments because 427 real-world networks with more than one million nodes. 482 we were unable to find adequate implementations. Also, 428 429 430 431 432 433 434 435 and q = 1).

436 $_{\rm 437}$ shared by the creators whenever possible. For classic $_{\rm 492}$ even be performed. ⁴³⁸ methods such as LE and Isomap, we use the implemen-⁴⁹³ 439 440 441 Python with the help of some open source packages. Note 496 and widely available implementations, and they yield de-442 that this is not the ideal setup for comparing the run- 497 cent performance in all tasks. The non-Euclidean embed-443 ning time of different methods since the programming 498 ding methods still present some challenges. Their non-444 language (see Table I) used can heavily affect the re- 499 Euclidean nature makes it non-trivial to incorporate their 445 sults and the implementation used in our experiments 500 results to common downstream tasks in general, which 446 can sometimes be further optimized. Instead, our ex- 501 may limit their applicability. Nevertheless, the fact that 447 periments mimic a more practical scenario where prac- 502 the non-Euclidean methods stand out in certain tasks 448 without spending too much time improving or even im- 504 ther investigation and improvement. 449 ⁴⁵⁰ plementing the methods themselves. The results here ⁴⁵¹ provide a rough estimation of the expected running time ⁴⁵² when using the most accessible implementation.

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DISCUSSION V.

In this work, we consider a large corpus of real-world 454 and synthetic networks, and measure the performance 455 of several embedding methods in solving specific net-456 work tasks. We find that Isomap and Node2vec outper-457 ⁴⁵⁸ form the other methods in greedy routing. As for link ⁴⁵⁹ prediction, community embedding, Mercator, and Hy-460 perLink all yield excellent performance. Our results on ⁴⁶¹ synthetic network models indicate that type and feature ⁵¹³ ⁴⁶² of the target networks are not important when choosing ⁴⁶³ the embedding method. Instead, one possible principle ⁵¹⁴ 464 is that the methods aim at preserving global network 515 that map the nodes of the input network into points in 465 structure excel in greedy routing, and methods only cap- 516 the target space. The coordinates of the nodes serve as 466 turing local information achieve optimal performance in 517 the vector representation of the networks and the pair-⁴⁶⁷ link prediction. Also, our analyses of the algorithm run- ⁵¹⁸ wise distance of different nodes correspond to their prox-⁴⁶⁸ ning time show that hyperbolic methods are much slower ⁵¹⁹ imity or similarity in the input networks. Depending on suited for embedding large-scale networks. 470

471 472 the decision of using an embedding method instead of 523 bedding methods by their target spaces, i.e., Euclidean, ⁴⁷³ another are measurable and quantifiable. Some methods ⁵²⁴ hyperbolic, and non-metric spaces.

⁴¹⁹ the hyperbolic embedding methods. When we apply the ⁴⁷⁴ may provide valuable insights into the characteristics of embedding algorithms to different network models and 475 networks although their performance may not be commeasure their computational time, results are qualita- 476 parable with that of others in certain tasks. For prac-477 tical tasks, many other features may also be crucial. A Among the methods tested, only Node2vec and com- 478 method can be chosen because its implementation is easy vain [24] and Infomap [25]) can easily scale up to large 400 ferent input networks. For instance, we had to exclude They complete the embedding in about 24 hours and 483 some of the methods considered in this paper require 1.4 hours, respectively, without compromising the per- 484 proper calibration of input parameters to be successful formance on downstream tasks (see details in Table IV). 485 in downstream tasks [12]. For example, choosing a large In order to avoid unnecessary memory and time usage 400 value for the embedding dimension for Node2vec, LE, while applying Node2vec on networks with millions of 487 and HOPE does not always lead to good results. These nodes, we use a program optimized for unweighted net- 400 methods can suffer from overfitting on certain tasks when works and specific algorithm parameter values (p = 1 489 the embedding dimension is too high. Calibration is gen-⁴⁹⁰ erally a computationally expensive operation, and there In our experiments, we try to use the implementation ⁴⁹¹ may be practical situations where calibration can not

All things considered, we believe that the Euclidean tation provided by the Python package scikit-learn [79]. 494 embedding methods like Node2vec and Isomap should be We implement Node2vec and community embedding in 495 the first options for practitioners since they have stable titioners hope to quickly apply the embedding methods 503 suggests that they have a great potential, calling for fur-

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VII. METHODS

Network Embedding Methods Α.

Network embedding methods are sets of procedures than other methods, suggesting that they are not yet well 520 the target spaces, the representation of the embedded ⁵²¹ network and the definition of the distance between nodes We stress that not all factors that are important in 522 in the embedding space vary. Here we group different em-

1. Euclidean embedding methods

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For Euclidean embedding methods, each node *i* can be 571 526 527 described by a *d*-dimensional vector $\mathbf{x}_i = (x_i^{(1)}, ..., x_i^{(d)})$ 528 where *d* is the space dimension and serves as a free pa-572 573 rameter for all Euclidean embedding methods. There 574 529 are several ways to calculate the distance between two 575 530 nodes in Euclidean embedding space. The most common 576 531 ⁵³² two, Euclidean distance and dot product, are used in this ⁵⁷⁷ 533 work. The Euclidean distance between node i and j is 578 534 defined as 579

dist_{ij} =
$$\|\mathbf{x}_i - \mathbf{x}_j\| = \sqrt{\sum_{v=1}^d (x_i^{(v)} - x_j^{(v)})^2}$$
. (2) 581
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535 The dot product between node i and j is given by

$$\mathbf{x}_{i} \cdot \mathbf{x}_{j} = \sum_{v=1}^{d} x_{i}^{(v)} x_{j}^{(v)} . \tag{3}$$

536 Note that the similarity between two vectors is propor-537 tional to their dot product. So we use

$$\operatorname{dist}_{ij} = -\mathbf{x}_i \cdot \mathbf{x}_j , \qquad (4)$$

⁵³⁸ as effective distance in the dot product approach.

591 Node2vec, LE, HOPE, and Isomap are the four Eu-530 592 ⁵⁴⁰ clidean embedding methods we consider in this paper. 593 We use either the distance of Eq. (2) or Eq. (4) depend-541 594 ing on the objective function that a method minimizes 542 595 and the actual downstream task. Eq. (2) is used for LE 543 596 and Isomap in this paper. For Node2vec and HOPE, 544 597 we use Eq. (4) for link prediction according to their ob-545 598 jective functions, and Eq. (2) for mapping accuracy and 546 greedy routing because it yields much better performance ⁵⁹⁹ 547 than when distance is calculated according to Eq. (4) (see $_{600}$ 548 Ref. [39], Sec. III). 549 601

Next, we briefly introduce each method and the parameters used in our experiments.

(1) Node2vec [20]: Node2vec first generates multiple ⁶⁰⁴ 552 node sequences using random walks with fixed 553 length, then finds the vector representations that 554 maximize the probability of co-occurrence of the 555 605 nodes in the sequences. There are some tunable 556 606 parameters for Node2vec, such as walk length l, 557 607 window size, the bias parameters of the random 558 608 walk dynamics p and q, and the embedding dimen-559 sion d. In this work, we use the default setting: 560 window size = 10, p = 1 and q = 1. 561

We find that the walk length can greatly affect different downstream tasks. The main reason is that 609 walk length directly control the type of information that the resulting embedding preserves. Short 611 walk lengths preserve local structural information; 612 long walk lengths preserve global structure. As expected, according to our tests on several real-world 614 networks, increasing the walk length improves the performance of mapping accuracy and greedy routing, but worsens link prediction (see Ref. [39], Sec. III). So we set l = 10 for link prediction and l = 100 for the other two tasks in this paper.

In general, the larger the dimension d, the better the embedding. But for Node2vec, the performance in downstream tasks may decrease slightly as d increases (see Ref. [39], Sec. III). In this work, we set $d = \min\{N, 128\}$ for all embedding methods that can work with high (d > 2) dimensional embedding space, which is considered a sufficiently high value to achieve nearly-optimal embeddings of networks [80]. We make this choice to maintain the simplicity of the experiments without introducing strong biases towards certain methods.

(2) Laplacian Eigenmaps (LE) [21]: LE aims to place the nodes that are connected with each other closely in the embedding space by minimizing the objective function

$$E_{\rm LE} = \sum_{ij} \|\mathbf{x}_i - \mathbf{x}_j\|^2 A_{ij} = tr(\mathbf{X}^T \mathbf{L} \mathbf{X}) , \qquad (5)$$

where $\mathbf{X} = (\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_n)^T$ is the low-dimensional representation matrix of the network, \mathbf{A} is the adjacency matrix of the network $(A_{ij} = A_{ji} = 1 \text{ if nodes}$ i and j are connected, otherwise $A_{ij} = A_{ji} = 0$), $\mathbf{L} = \mathbf{K} - \mathbf{A}$ is the Laplacian matrix and \mathbf{K} is the diagonal matrix with $K_{ii} = \sum_j A_{ji}$. LE further requires $\mathbf{X}^T \mathbf{K} \mathbf{X} = \mathbf{I}$ to eliminate trivial solutions. To obtain a d-dimensional embedding, one can simply extract the eigenvectors that correspond to the d smallest non-zero eigenvalues of the solution to $\mathbf{L} \mathbf{x} = \lambda \mathbf{K} \mathbf{x}$.

LE only has one tunable parameter: dimension d. We set it to $d = \min\{N, 128\}$.

(3) HOPE [22]: Given a node similarity definition, HOPE seeks to preserve the similarity matrix S in the embedding space by minimizing

$$E_{\text{HOPE}} = \|\mathbf{S} - \mathbf{x}\mathbf{x}^T\|,\tag{6}$$

through singular value decomposition (SVD). HOPE can work with different node similarity definitions; here we use Katz index, which is calculated by

$$\mathbf{S}^{\text{Katz}} = \beta \sum_{l=1}^{\infty} \mathbf{A}^l , \qquad (7)$$

where **A** is the adjacency matrix of the network and β is the decay parameter. HOPE requires $\beta < 1/\lambda_{max}$, with λ_{max} principal eigenvalue of the matrix **A**. We set $\beta = 1/\lambda_{max} - 0.001$ for all experiments. The embedding dimension *d* is set to $d = \min\{N, 128\}$.

(4) Isomap [23]: Isomap tries to preserve the short- 655 615 est path distance between each pair of nodes. It 656 616 first calculates the shortest path distance matrix 657 617 **D** of a network. Then multidimensional scal-658 618 ing (MDS) [81] is applied to \mathbf{D} to obtain a d-659 619 dimensional representation of the network that 660 620 minimize the stress function 661 621

$$E_{\rm ISO} = \sum_{ij} \left[D_{ij} - \| \mathbf{x}_i - \mathbf{x}_j \| \right]^2 . \tag{8}$$
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We set the embedding dimension $d = \min\{N, 128\}$ 665 622 for Isomap in all experiments. 666 623

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2. Hyperbolic embedding methods

For hyperbolic embedding, nodes are usually consid-671 625 672 ered as points on the Poincaré disk. Two coordinate sys-626 tems are often used in the literature, i.e., the polar coordi-673 627 628 nates (r, θ) and the Poincaré coordinates $\mathbf{y} = (y^{(1)}, y^{(2)})$. 674 675 The Poincaré coordinates are similar to the Euclidean 629 676 coordinates but represent points in hyperbolic space. 630 677 They can also be extended to arbitrary dimension, i.e., 631 $\mathbf{y} = (y^{(1)}, \dots, y^{(d)})$, to represent points in the Poincaré 678 632 679 ball. 633

When using the polar coordinates, the distance be-680 634 681 tween node i and j can be calculated by 635 682

$$\operatorname{dist}_{ij} = \operatorname{arcosh}(\operatorname{cosh} r_i \operatorname{cosh} r_j - \operatorname{sinh} r_i \operatorname{sinh} r_j \operatorname{cos}(\Delta \theta)), \quad {}^{683}_{684}$$

$$(9) \quad {}^{684}_{684}$$

where $\Delta \theta = \pi - |\pi - |\theta_i - \theta_j||$ is the angle between the 636 685 two nodes. 637 686

When using the Poincaré coordinates, the distance be-638 $_{639}$ tween node *i* and *j* can be calculated by

$$\operatorname{dist}_{ij} = \operatorname{arcosh}\left(1 + 2\frac{\|\mathbf{y}_i - \mathbf{y}_j\|^2}{(1 - \|\mathbf{y}_i\|^2)(1 - \|\mathbf{y}_j\|^2)}\right). \quad (10) \quad {}^{689}_{691}$$

The two-dimensional Poincaré coordinates $(y^{(1)}, y^{(2)})$ 640 693 and the polar coordinates (r, θ) of hyperbolic space can 642 be converted to each other by 694 695

$$r = 2 \operatorname{artanh}(\sqrt{(y^{(1)})^2 + (y^{(2)})^2}), \qquad (11) {}^{696}_{697} \\ \theta = \operatorname{atan2}(y^{(2)}, y^{(1)}). \qquad (12) {}^{696}_{697}$$

Among the hyperbolic embedding methods consid-699 643 644 ered in this work, HyperMap, Mercator, and Hyper- 700 Link use polar coordinates; Poincaré maps and Hydra 701 645 use Poincaré coordinates. Poincaré maps focus on the 646 702 two-dimensional disk while Hydra can embed networks 703 647 in higher-dimensional hyperbolic spaces. 704 648

We briefly introduce each method and the parameters ⁷⁰⁵ 649 used in our experiments in the following. 706 650

(1) HyperMap [13,19]:Popularity-similarity- 708 651 optimization (PSO) model [4, 19] is a growing 709 652 network model that can simultaneously capture 710 653 the heterogeneity degree distribution and the 711 654

strong clustering structure of real-world networks. Nodes of PSO model are embedded in hyperbolic space and their coordinates have clear interpretations: the radial coordinate represent the node popularity, and the difference between angular coordinates of a node pair represents the similarity The PSO model consists of a between them. probability law for the existence of edges between pairs of nodes in the network depending on their distance in the hyperbolic space, i.e., Eq. (9).

As an embedding method, HyperMap embeds an input network to the hyperbolic space by fitting the network against the PSO model. The fit is performed by maximizing the likelihood of observed edges according to the PSO connection probability law. As the maximum likelihood problem cannot be solved exactly, different variants of the HyperMap algorithm exploit different strategies to find approximate solutions. These variants include the link-based method [19], the commonneighbors based method (also called HyperMap-CN) [13], and the hybrid method [13] that uses the common-neighbors based method for high degree nodes and the link-based method for the rest of the nodes. The computational complexity of the abovementioned algorithms is at least $O(N^3)$. There is also a speed-up version of the hybrid method, which can reduce the computational complexity of the method down to $O(N^2)$ without compromising the embedding quality too much.

In this paper, we use the speed-up version of HvperMap. This method has extra correction steps that can marginally improve the results but have a very high computational complexity so we disable them. It has a parameter k_{speedup} to control the level of acceleration. We set $k_{\text{speedup}} = 10$ for networks with size N < 10,000 and $k_{\text{speedup}} = 40$ for networks with size N > 10,000.

The input parameters of HyperMap include the temperature $T \in [0, 1)$, which reflects the average clustering level of a network. A higher temperature means that the network is less clustered. Identifying the ideal temperature value for each network requires scanning the parameter space, which is infeasible in our experiments. Instead, we test the overall performance of HyperMap for different values of the temperature parameter on several realworld networks and find that temperatures that are not too large nor too small generally yield decent performance (see Ref. [39], Sec. III). So we set temperature T = 0.5 in all experiments. Another input parameter of HyperMap is the exponent $\gamma \geq 2$ of the power-law degree distribution of the network. Note that not all real-world networks display a power-law degree distribution. To apply HyperMap to all the networks considered, we use the code shared by Broido et al. [82] to estimate a

- suitable γ value for every network. If the estimated 768 712 γ value is smaller than 2.1, we set $\gamma = 2.1$. 713
- (2) Mercator [14]: Mercator learns the hyperbolic rep-714 resentations of networks by matching them with 715 the $\mathbb{S}^1/\mathbb{H}^2$ model [83, 84]. The $\mathbb{S}^1/\mathbb{H}^2$ model is the 716 static version of the PSO model. While PSO model 717 can only generate networks with pure power-law 718 degree distribution, the $\mathbb{S}^1/\mathbb{H}^2$ model can generate 719 networks with arbitrary degree distributions. Be-720 sides the input network itself, Mercator does not 721 require any input parameters. 722
- (3) Poincaré maps [15]: Poincaré maps aims to pre-723 724 Isomap. 725 Poincaré maps. For example, the Gaussian kernel $_{782}$ b in the supernetwork is defined as 726 width σ_P is related to the calculation of the global 727 proximity of the original network, the scaling pa-728 rameter γ_P is used to tune the scattering of the 729 embedding. We find that these parameters have 730 little effect on the results. In this paper, we use 731 the default setting $\sigma_P = 1$ and $\gamma_p = 2$ in all exper-732 iments. The maximum number of epochs for the 733 embedding optimization is set to e = 1000. 734
- (4) Hydra [16]: Like Poincaré maps and Isomap, Hy-735 dra (HYperbolic Distance Recovery and Approx-736 imation) also seeks to preserve pairwise shortest 737 path length. The difference between Poincaré maps 738 and Hydra is that Hydra can work in hyperbolic 739 spaces of arbitrary dimension, while Poincaré maps 740 is designed for the two-dimensional space only. The 741 dimension d is the only one free parameter of Hy-742 dra. We set $d = \min\{N, 128\}$ in all experiments. 743
- (5) HyperLink [17]: HyperLink is a model-based hyper-744 bolic embedding method designed for link predic-745 tion. It tries to fit the networks to the random hy-746 perbolic graphs (RHGs) model, which is equivalent 747 to the $\mathbb{S}^1/\mathbb{H}^2$ model used in Mercator. HyperLink 748 assumes that a fraction p of links are missing when 749 embedding a network. In addition to p, other in-750 put parameters of HyperLink include the exponent 751 $2 < \gamma < 3$ of the degree distribution, the tempera- 798 even though \bar{f}_{ij} is not a proper metric of distance. 752 ture T, the number of layers m, and the coefficient 753 g that controls the size of the mesh in the angular 754 space. In our experiments, we use the default set-755 tings m = 20 and g = 1. We aid the method by 756 setting p = 0.3 in link prediction, and p = 0 in other 800 757 758 759 760 761 762 763 764 765 766 our experiments. 767

Non-metric embedding method 3.

Community embedding [18] is a non-metric embedding 769 ⁷⁷⁰ method inspired by the analogy between hyperbolic em-⁷⁷¹ beddings and network community structure. It embeds 772 networks using information about their community struc-⁷⁷³ tures: node *i* is represented by the coordinates (k_i, σ_i) where k_i is node's degree and σ_i is the index of the 774 775 community that the node belongs to. There are many 776 community detection algorithms available on the market. ⁷⁷⁷ Here, we use two popular ones: Infomap [25] and Lou-⁷⁷⁸ vain [24]. After the community partition of a network 779 is obtained, nodes in the same communities are merged serve the pairwise shortest path length just like 780 together to generate supernodes, which then form a su-There are several free parameters of $_{761}$ pernetwork. The edge weight between community a and

$$w_{ab} = 1 - \ln \rho_{ab}$$
, if $\rho_{ab} > 0$, (12)

783 and $w_{ab} = 0$, otherwise. ρ_{ab} is the ratio between the total $_{784}$ number of edges between communities a and b and the $_{785}$ sum of the node degrees in community *a*.

The fitness between nodes j and i is defined as

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$$f_{ij} = \beta D_{\sigma_i \sigma_j} - (1 - \beta) \ln k_i , \qquad (13)$$

787 where $D_{\sigma_i \sigma_j}$ is the shortest path length between commu-788 nities σ_i and σ_j in the supernetwork, k_i is the degree of 789 node *i*, and $0 \leq \beta \leq 1$ is a free parameter. In order ⁷⁹⁰ to maximize the overall performance of community em-⁷⁹¹ bedding on different tasks, we test the effect of β for the ⁷⁹² tasks on some real-world networks, and set $\beta = 0.3$ for all ⁷⁹³ experiments (see Ref. [39], Sec. III). Note that the fitness ⁷⁹⁴ of Eq. (13) is an asymmetric function, i.e., $f_{ij} \neq f_{ji}$. In ⁷⁹⁵ this paper we symmetrize it as

$$\bar{f}_{ij} = \frac{f_{ij} + f_{ji}}{2},\tag{14}$$

796 and we treat it at the same footing as of a distance be-⁷⁹⁷ tween nodes i and j, i.e.,

$$\operatorname{dist}_{ij} = \bar{f}_{ij} \,, \tag{15}$$

Networks В.

In this paper, we use both real-world networks and tasks. The estimation of γ is the same as in Hyper- $_{801}$ synthetic networks. All networks are unweighted and Map. We set $\gamma = 2.1$ if the estimated $\gamma < 2.1$ and $_{802}$ undirected. We consider 72 real-world networks from dif- $\gamma = 2.9$ if the estimated $\gamma > 2.9$ in order to satisfy $_{303}$ ferent domains, including social, biological, technological, the requirement. Like HyperMap, the temperature and transportation, and Internet networks. Sizes of these net-T is a free parameter for HyperLink. We test the $_{005}$ works ranges from 32 to 37,542 nodes. Figure 7 shows overall performance of HyperLink for different T_{806} the average degree versus network size for all the 72 realvalues on some real-world networks, and find that ⁸⁰⁷ world networks used. Two networks with more than one T = 0.3 yields the best performance overall (see 100 million nodes are also considered for Node2vec and com-Ref. [39], Sec. III). Therefore, we set T = 0.3 in ⁸⁰⁹ munity embedding particularly to demonstrate their scal-⁸¹⁰ ability. The full list of the real-world networks and some



FIG. 7. Summary statistics of the real-world networks ⁸⁵² considered in this study. In the main panel, we show the ⁸⁵³ scatter plot of the average degree $\langle k \rangle$ versus network size N. ⁸⁵⁴ Each point is a real network in our dataset. Side panels are used to display non-normalized distributions of $\langle k \rangle$ and N.

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⁸¹¹ of their basic information can be found in Ref. [39], Sec. ⁸¹² I. Only the largest connected component of the various ⁸¹³ network is considered in our analysis.

We use 34 synthetic networks generated according to different models. We ensure that each network instance consists of one connected component only. The network models considered are reported below.

(1) Popularity-similarity-optimization (PSO) model [4, 866 818 19]: PSO model grows networks by adding nodes ⁸⁶⁷ 819 to a hidden hyperbolic space. Nodes close with 868 820 each others in the hidden space are then connected 869 821 to form the edges. There are several parameters ⁸⁷⁰ 822 that could affect the properties of the generated 871 823 networks: network size N, temperature T, aver- ⁸⁷² 824 age degree $\langle k \rangle$, and exponent γ of the power-law ⁸⁷³ 825 degree distribution $P(k) \sim k^{-\gamma}$. Temperature $T \in {}^{874}$ 826 [0, 1) controls the average clustering in the network, ⁸⁷⁵ 827 which is maximized at T = 0. We generate six in-828 stances of the PSO model with the following pa- 877 829 rameters: $N = \{1000; 10, 000\}, T = \{0.1; 0.5; 0.9\}, 878$ 830 $\gamma = 2.1, \langle k \rangle = 5.$ 831

- (2) Lancichinetti-Fortunato-Radicchi (LFR)model [76]: The LFR model generates networks with community structure, and both the degree distribution P(k) and community size distribution P(S) follow power-law distribution, i.e., $P(k) \sim k^{-\gamma}$ and $P(S) \sim S^{-\tau}$. Input parameters that are required to generate instances of the model are the network size N, the exponents γ and τ , the average degree $\langle k \rangle$, the maximum degree k_{max} , the minimum and maximum community size c_{\min} and $c_{\rm max}$, and the mixing parameter μ that determines how strong the community structure is. A small value of μ corresponds to a strong community structure. We generate eight instances of LFR models, the parameters are $N = \{1000; 10, 000\},\$ $\mu = \{0.1; 0.3; 0.5; 0.7\}, \ \gamma = 2.1, \ \tau = 2, \ \langle k \rangle = 5,$ $k_{\text{max}} = 50, c_{\text{min}} = 10, c_{\text{max}} = 0.1N.$
- (3) Poisson networks: They are generated by feeding Poisson degree distributions to the configuration model. Two tunable parameters are the size of network N and average degree $\langle k \rangle$. We use eight instances of Poisson networks with the following parameters: $N = \{1000; 10, 000\}, \langle k \rangle = \{4; 6; 8; 10\}.$
- (4) Power-law networks: They are generated by feeding power-law degree distributions to the configuration model. The tunable parameters are the network size N and the power-law exponent γ . The average degree of a network can be controlled by setting the minimum value of the node degrees, namely k_{\min} . We use six instances of power-law networks and the parameters are N = $\{1000; 10, 000\}, \gamma = \{2.1; 2.5; 2.9\}, k_{\max} = 100$. We use either $k_{\min} = 2$ or $k_{\min} = 3$ for nodes in the network to ensure an average degree $\langle k \rangle \simeq 5$.
- (5) Spatial networks [77]: The model generate spatial networks that are embedded in two-dimensional regular lattice. Both the degree distribution P(k) and the Euclidean distance distribution of edges P(r) follow power-law distributions, i.e., $P(k) \sim k^{-\gamma}$ and $P(r) \sim r^{-\alpha}$. The input parameters of the model are the network size N, the exponents γ and α , the minimum and maximum degree k_{\min} and k_{\max} . We use six instances of the model, with parameters chosen as $N = \{1000; 10, 000\}, \gamma = \{2.1; 2.5; 2.9\}, \alpha = 2, k_{\max} = 100$. We use either $k_{\min} = 2$ or $k_{\min} = 3$ for nodes in the network to ensure an average degree $\langle k \rangle \simeq 5$.
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