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1 Measuring Polycentricity: A Whole Graph 2 Embedding Perspective

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15 — Abstract —

16 Polycentricity is a critical characteristic of the spatial organization of cities. Many indices have
17 been proposed to measure the degree of morphological polycentricity or functional polycentricity.
18 However, selecting a proper set of polycentricity indices for cities in a particular region or country
19 still needs prior expert knowledge. This study demonstrates that whole graph embedding, as a novel
20 and efficient computational tool, can model the city polycentricity in an integrated manner without
21 much prior knowledge. The new method can further support visual analytics and classification very
22 well.

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30 innovation program under grant agreement No 780754.

31 **1** Introduction

32 Polycentricity is a spatial organization of a city such that the city's socio-economic functions
33 are shared by the traditional central business center (CBD) with subcenters. The spatial
34 organization has complex social and environmental impacts. Highly polycentric cities are
35 found to reduce household CO₂ emission but increase transportation emission in the US
36 [12]. The spatial organization of a city can be conceptualized as a combination of the
37 spatial distribution of its residents and their trip patterns [3]. There have been many indices
38 to measure polycentricity either from the morphological polycentricity perspective, which
39 measures the spatial distribution of the residents, or from the functional polycentricity
40 perspective, measuring e.g. the transportation patterns [9, 13]. Although polycentricity can
41 be interpreted in many different ways, transportation patterns usually form the research
42 focus [6]. Many indices partially utilize graph analysis to model the transportation data

43 and extract graph features, such as network density. However, these indices do not achieve
44 consistent conclusions for the same cities of different countries in empirical studies [2].

45 Whole graph embedding is a network analysis technique that maps graphs with different
46 sizes and structures into a Euclidean vector space, namely an *embedding space*, so that each
47 graph is represented as a node in the embedding space, namely an *embedding vector*, and
48 similar graphs are located close in the embedding space [5]. As some whole graph embedding
49 methods can represent both edge features and node features in the same representative node,
50 they have the potential to be used as a tool for measuring the city polycentricity combining
51 both the spatial distribution of the residents and the transportation patterns.

52 This study thus explores the following research question: *Can whole graph embedding*
53 *differentiate cities with different polycentricity?* To answer this research question, we
54 select a proper whole graph embedding model and apply the model to transportation data
55 from artificial cities and a real-world city.

56 **2 Related Work**

57 **2.1 Conventional Polycentricity Indices**

58 There are three main groups of polycentricity indices [13]: The first is rooted in social graph
59 analysis, such as using nodality and centrality as the focal metric and using the degree of
60 the standard deviation of a city's metric from a maximum possible standard deviation value
61 as the metric. For example, [9] uses the total volume of inflow traffic to a place as the
62 metric and [13] uses the centrality as the metric. The second group relies on the slope of
63 the size-rank distribution of a specific feature, e.g., population or inflow traffic volume to a
64 place, to measure the polycentricity, such as [14, 4]. The third group compares the real-world
65 observation of a metric to an ideal model to measure the degree of polycentricity, e.g., [1]
66 uses the average commute distance. All these methods use a highly aggregated statistical
67 metric, but each of these metrics can only describe a single perspective of the transportation
68 network, which misses out on many complex patterns. As an empirical study of Polish cities
69 shows, the indices are not consistent, meaning that contradictory conclusions can be made
70 for the same city [2]. [7] further discuss the issue of inconsistencies and propose that further
71 exploration of polycentricity should take multiple critical factors into account, including the
72 concepts of centers, polycentricity, geographical context, and more. Multiple metrics should
73 be applied to see if the results are consistent. That means researchers should already have
74 sufficient knowledge about the dynamics of their study subjects. Therefore the workflow can
75 hardly be applied to a study covering many cities or over several regions or countries that
76 have different geographical contexts.

77 **2.2 Whole Graph Embedding Models**

78 There are several groups of technical solutions to embed a whole graph. The first group is
79 graph-kernel-based, such as graph2vec [15], inspired by doc2vec [11], by combining a shallow
80 neural network with inputs sampled from random walks through the graphs. The second
81 group applies deep learning architectures such as conventional neural networks [10, 16]. The
82 third group utilizes spectral representation [17]. Different whole graph embedding methods
83 are specialized to model directed/undirected or weighted/binary graphs, with/without node
84 properties for different scenarios. Some are designed for downstream classification tasks,
85 meaning that a classifier is required as part of the modeling. In contrast, others can be used
86 for dimension reduction, where no training process is needed.

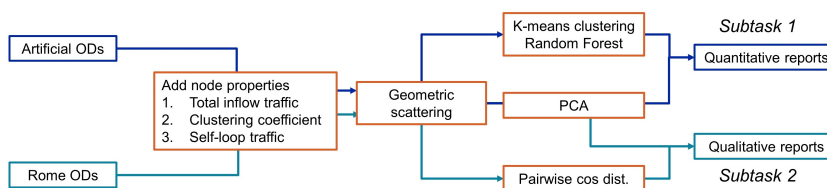


Figure 1 Overall analytical workflow

3 Methodology

To examine if the whole graph embedding method can differentiate cities with different degrees of polycentricity, we applied the method to a set of origin-destination (OD) graphs as artificial cities designed by [2] and the hourly OD graph of Rome. We conducted two subtasks (Figure 1): For the artificial cities, we applied the modeled embedding vectors as input of a classification task and a clustering task, respectively, to quantitatively examine if the embedding vectors of the cities are differentiable, denoted as Subtask 1. For the OD graphs of Rome, we applied visual analytics to investigate if the patterns of embedding vectors fit the existing knowledge and provide new knowledge, denoted as Subtask 2.

3.1 Data Collection and Preprocessing

The *original* artificial cities consist of OD matrices of six cities: three cities have five nodes as places and three cities have ten nodes. The three cities with the same number of nodes are designed as *extremely polycentric*, *intermediate*, and *extremely monocentric*, respectively. *Extended* artificial cities are made by an augmentation process using each original artificial city as a template: For each pair of two nodes, there is a possibility (denoted as PROP) to add an additional traffic volume ranging from one to a maximum volume (denoted as MAX_WEIGHT) to the template city to make a new city. By controlling the value of PROP and MAX_WEIGHT, we were able to generate new artificial cities with a similar polycentricity as their template with slightly different node and edge features. Each template city was augmented into five new cities.

The real-world OD graphs were derived from big vehicle trajectory data recorded in 2017. We only considered the origin and destination of a trip, discarding any passing-by stops. The origins and destinations were tessellated into 1-km grids and aggregated by every hour. The hourly OD traffic volumes of the year were further averaged into 24 OD graphs.

3.2 Whole Graph Embedding and Analytics

The whole graph algorithm used in this study is a geometric-scattering-based algorithm by [8]. Essentially, the algorithm applies cascading multi-layer wavelet transforms to a graph to extract scattering features. This algorithm is able to model the embedding of weighted directed graphs with node properties, which is suitable to model the OD graphs as we would like the model to describe the structural information of the transportation network and the properties of the origin and destination locations such as their demographics holistically. This algorithm is also not specialized for classification tasks as it does not require labeled data. Thus, the algorithm is suitable for exploratory tasks.

In this study, we used the traffic volume of the OD graph as the edge feature. In addition, we used the total volume of inflow traffic, self-loop traffic volume, and the clustering coefficient

122 as the node features. Self-loop traffic volume acts as a proxy for the residential population of
 123 the place. The clustering coefficient measures how a place and its neighboring places cluster
 124 topologically, which is also used in the original study [8].

125 For Subtask 1 involving the artificial cities, as we already knew the label of the tem-
 126 plates, we explored how the values of PROP and MAX_WEIGHT influence the results of
 127 the whole graph embedding. We hypothesized that with increasing values of PROP and
 128 MAX_WEIGHT, the extended cities might be more different from their template city in
 129 terms of their patterns. Exploring the locations of the extended cities and their corresponding
 130 template cities in the embedding space can also examine the sensitivity of the embedding
 131 algorithm towards small changes of the cities. We used principal component analysis (PCA)
 132 to visually interpret the embedding results. The PCs that cumulatively explain 90 % vari-
 133 ability were kept. Then, we passed the embedding vectors to k-means clustering to check
 134 if the clustering method can differentiate cities with different polycentricity types, using
 135 the silhouette score as the metric. We also passed the embedding vectors as the features
 136 for training and used 5-fold cross-validation on random forests to examine the classification
 137 results, using average accuracy as the metric. For Subtask 2 on the Rome hourly OD graphs,
 138 we applied visual analytics using PCA and the pairwise cosine distance to understand the
 139 patterns of the embedding vectors and explored the influence of residents' trip patterns at
 140 different times on the embedding outputs given the fixed morphological polycentricity.

141 4 Results

142 As the PCA transformed visualization shows (Figure 2.a), cities with different polycentricity
 143 degrees can be differentiated visually: The extremely polycentric cities take the lower-left
 144 corner. The cities with extremely monocentric cities take the lower-right, and the intermediate
 145 cities take the upper region. For the k-means clustering (Figure 2.b), there will be five
 146 clusters using PCA-transformed vectors as input features and using the maximum value of
 147 silhouette score as the criterion to pick the best k . The best solution with $k = 5$ is almost
 148 the same as the six-type ground truth without prior knowledge of the labels. It can also be
 149 observed that the silhouette scores of specific k -values using PCA-transformed vectors are
 150 even higher than the score of ground truth labels, which might be due to the noise added
 151 during the augmentation. A similar influence of added noise can also be observed in Figure
 152 2.a: some points are far from their templates, such as ip_ten_3 and em_five_0. From the
 153 classification results regarding the PROP ranging from 0.1 to 0.7 and the MAX_WEIGHT
 154 ranging from 1 to 10 (Figure 2.c and d), it can be observed that the artificial cities are still
 155 easy to be differentiated, while the average accuracies are almost all above 0.80. Combining
 156 the results of the three methods, it can be summarized that whole graph embedding using
 157 geometric scattering can differentiate the degree of polycentricity of the artificial cities.

158 For the per-hour traffic graphs of Rome, both PCA visualization and the pairwise cosine
 159 distance matrix (Figure 3) suggest the existence of three clusters, one ranging from 02:00 to
 160 07:00, a second one from 08:00 to 11:00, and the third one from 14:00 to 18:00. The pairwise
 161 cosine distance matrix further suggests that the graphs have a clear temporal autocorrelation
 162 with their neighboring hours for most cases. This observation generally fits the common-sense
 163 perception of the commuting patterns of a city: The first and third clusters might correspond
 164 to more polycentric patterns for diverse mobility, while the second cluster might be more
 165 monocentric, corresponding to commuting hours. However, as the per-hour traffic flows do
 166 not differentiate between weekdays, weekends, and holidays so far, the patterns still need
 167 further validation. In addition, although the embedding vectors cannot provide a simple

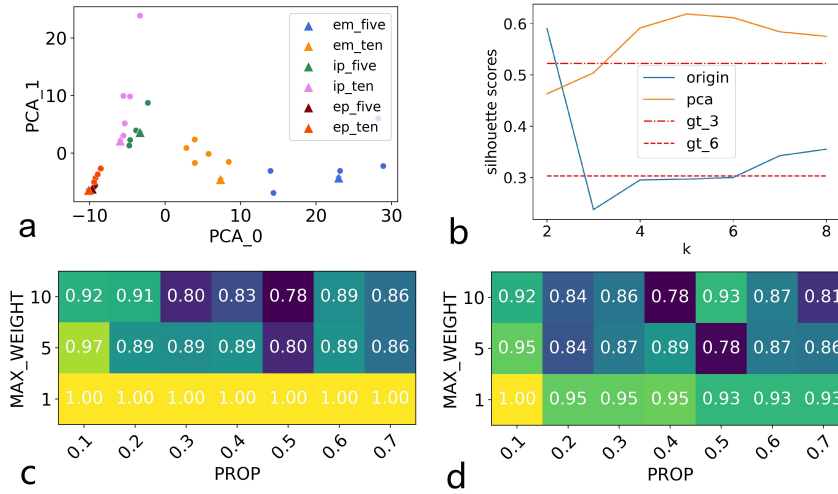


Figure 2 a) The PCA transformed embedding vectors of the six original artificial cities. The first principal component takes 66.2% of the overall variation, and the second principal component takes 20.3%. em: extreme monocentric; ip: intermediate; ep: extreme polycentric. Extended cities are points sharing the same color with their template cities. b) The silhouette scores against different k values. gt_3: using the three city types as the ground truth labels. gt_6: using the combinations of city type and city size (6 labels) as ground truth. c) The average accuracy of 5-fold cross-validation of the classification of the three city types against the PROP and MAX_WEIGHT on the extended artificial cities (36 cities). d) The average accuracy of 5-fold cross-validation of the classification of differentiating the combinations of city type and city size against the PROP and MAX_WEIGHT.

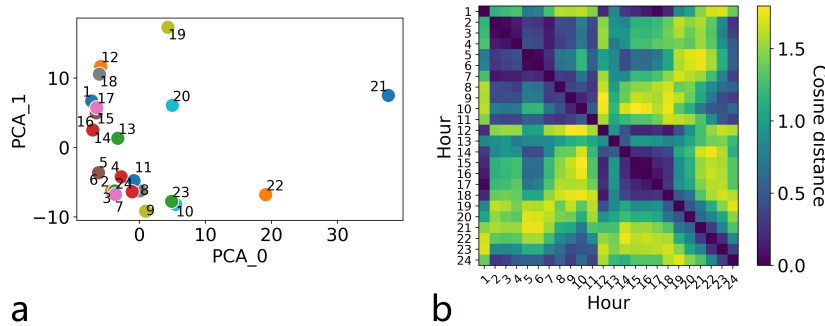


Figure 3 a) The PCA-transformed embedding vectors of per hour traffic graphs of Rome. Point colors are randomly assigned. b) Pairwise cosine distance of the embedding vectors.

168 and absolute scale for the polycentricity, as other existing statistical metrics do, the relative
 169 relationships can still be interpreted from the distance matrix. Nevertheless, the results still
 170 show the capacity of whole graph embedding as an analytical tool.

171 **5 Conclusion and Future Work**

172 Whole graph embedding is able to model the complex structure information of graphs and
 173 represent the non-Euclidean graphs in a distributed way in a Euclidean space that benefits
 174 a lot of analytical tools. With two preliminary experiments of applying a whole graph

175 embedding algorithm to artificial traffic flow graphs and real-world traffic flow graphs, we
 176 demonstrated that the selected whole graph embedding algorithm is able to represent a
 177 complex traffic graph as an embedding vector. The embedding vectors of the cities can
 178 differentiate polycentricity through visual analytics tools and machine learning algorithms.

179 Although the preliminary results are encouraging, there are still questions remaining that
 180 need to be addressed in future work. For example, what node features are the best for mod-
 181 eling polycentricity; and how do morphological polycentricity and functional polycentricity
 182 contribute to the embedding vectors, respectively?

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