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Hierarchical graph embedding in vector space by graph pyramid

Seyedeh Fatemeh Mousavi, Mehran Safayani*, Abdolreza Mirzaei, Hoda Bahonar

Department of Electrical and Computer Engineering, Isfahan University of Technology, Isfahan 84156-83111, Iran

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ABSTRACT

Loss of information is the major challenge in graph embedding in vector space which reduces the impact of representational power of graphs in pattern recognition tasks. The objective of this article is to present a hierarchical framework which can decrease this loss in a reasonable computational time. Inspired by multi-resolution ideas in image processing, a graph pyramid is formed based on a selected graph summarization algorithm which can provide the required information for classification. All the pyramid levels or some of them are embedded into a vector through an available embedding method which constructs an informative description containing both local and global features. The experiments are conducted on graphs with numerical and categorical attributes. In the numerical case, a proposed summarization algorithm is applied while in the categorical case, *k*-SNAP graph summarization is applied. The results indicate that this new framework is efficient in terms of accuracy and time consumption in the context of classification problems. It is observed that this improvement is achieved regardless of selected embedding techniques.

1. Introduction

The superior representational power of graphs introduces these data structures as popular replacements for vectors in many pattern recognition applications. Lack of algorithmic tools is one of the main drawbacks of the graph structure. To overcome this drawback, graph embedding in vector space [1–7] provides the opportunity to benefit from the rich repository of vector based methods which are the results of many years of research and experience. However, the problem of finding appropriate vector representations for graphs is not an easy task. Two issues concern embedding methods: first, embedding procedures should not include costly operations and second, extracted features should preserve graph information, the structural details in particular as much as possible. These opposite requirements become more remarkable in larger and more complex graphs. In fact, with growing size of a graph, the cost of extracting useful information from all its components increases. Moreover, the augmented structural complexity raises the possibility of noise and distortion in structure and content of the original graph and this phenomenon makes the feature extraction more critical. As a result, in order to obtain a vectorial representation of a graph, a compromise between the embedding time and the ability of preserving information must be established, with respect to application. To accomplish this objective, a hierarchical framework is introduced in this article.

Multi-resolution processing is employed successfully in computer vision and image processing algorithms. This method tries to simulate the main characteristics of human visual perception [8]. For this purpose, the applied data structure should be able to represent both the distributed local information of the raw data and the hidden global information within. This structure is named the hierarchical architecture [9] the general scheme of which is shown in Fig. 1. It is observed that this hierarchical structures can be applied to efficiently extract the global information (image interpretations) from the local ones (array of pixel intensities) in a recursive manner. This structure provides an appropriate manner in order to cope with the limitations of memory and time and is considered as a bridge between local information and global interpretation.

In the notion of the hierarchical structure, the graphs are very similar to the images, that is, although the local processing through checking labels and adjacency relations can provide useful information about the content of the graph, accurate understanding of the global graph information requires the processing of substructures in different scales. This processing may be more important in matching and classifying large graphs, since the effective features cannot be detected merely with visual inspection and they can occur in every scale. Depending on the application, the similarities on one or all the scales may be of interest.

* Corresponding author.
E-mail addresses: sf.mousavi@ec.iut.ac.ir (S.F. Mousavi), safayani@cc.iut.ac.ir (M. Safayani), mirzaei@cc.iut.ac.ir (A. Mirzaei), h.bahonar@ec.iut.ac.ir (H. Bahonar).

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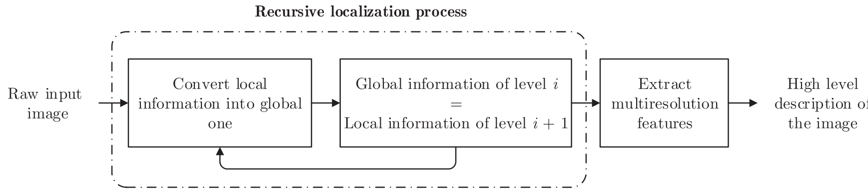

Fig. 1. A general scheme of hierarchical architecture in image processing. A recursive process is run to localize information in lower levels and extract global and informative features from higher levels. The selected features from all or some levels provide a useful description about the input image.

Therefore, the processing at different scales is necessary in the graph domain. Accordingly, transferring the concept of image pyramid to the graph domain can be beneficial.

Based on this idea, this article introduces a framework named *pyramidal graph embedding (PyrGE)* the objective of which is to provide easy access to a variety of information of the graph hierarchy and to apply them in reducing the missing information during embedding. It is expected that this framework increases the classification accuracy by reducing the complexity of managing large graph data. In this approach, a graph summarization algorithm [10,11] is employed as an operator for graph data localization in different scales. The graphs of different levels are embedded into the vectors using the single scale embedding methods and the obtained vectors are combined into a single vector.

In brief, the main contribution of this article is to apply an extracted hierarchical graph set rather than just applying the original graph for embedding in order to extend the representational power of the obtained embedded graph. The proposed framework is generic enough to handle different types of graphs provided that proper graph summarization and embedding methods are adapted to the type of graphs. In order to show this adaption, the experiments are run on three datasets, the first two datasets contain numerical node labels and last one contains categorical node label. For the numerical datasets, a new summarization procedure appropriate for this kind of graphs is proposed while for the categorical dataset, an existing summarization method, *k*-SNAP [11] is applied. The main achievement of this assessment is that regardless of the selected embedding method for each level, embedding procedure through this proposed hierarchical architecture improves the classification accuracy in all experiments in a significant manner.

The outline of this paper is organized as follows. The literature review is presented in Section 2; the primary concepts are discussed in Section 3; the details on how graph pyramid can be applied to enhance the existing embedding methods is expressed in Section 4; the design of several scenarios with respect to this framework is presented in Section 5; the concluding remarks and future works complete this article in Section 6.

2. Literature review

2.1. Graph embedding

The embedding methods can be divided into three groups based on their feature extraction approach. The first group is inspired by dissimilarity representations proposed in [12]. Riesen and Bunke [1] present the vectorial description of a graph by its distances to a number of prototype graphs. The second group is based on the frequencies of appearance of some specific knowledge-dependent substructures, capturing topology information and content of graph through its labels. This group is known as graph probing based methods [13]. For example, in [14] the vector is built by counting the occurrences of non-isomorphic model graphs included in the target graph. The recent approach of Gibert et al. [2] is based on different statistics on the node labels and the edge relations among them. Luqman et al. [3] consider the graph information in several levels of topology, structure and attributes. The third group, the spectral graph embedding, is a prominent group based on feature extraction from eigen-decomposition of adjacency or Laplacian matrices [15,4]. For example, Ren et al. [5] extracted cycle frequencies as the graph features through the Ihara Zeta function. Aziz et al. [6] applied backtrackless walks to capture the path and cycle information by avoiding tottering.

Each one of these groups has some drawbacks, which become more apparent in the case of large graphs. Dissimilarity-based methods (group 1) are able to handle arbitrary graphs and cope with structural distortions due to the use of graph edit distance as the basic dissimilarity measure. However, its computational cost is a challenge in dealing with large graphs. Probing based methods (group 2) are capable of using specific domain knowledge by finding substructures, but this procedure has high computational cost of subgraph isomorphism. Newer probing-based methods rely more on labels and binary relations and somewhat ignore the complex substructures of relatively large graphs. The spectral methods (group 3) provide intriguing and meaningful properties of a graph with polynomial time complexity, while they have the built-in problem of sensitivity to noise and are restricted to graphs with strongly limited label alphabets.

2.2. Pyramidal models

A wide range of applications such as image segmentation [16], region description and detection [17] make use of pyramid as a useful structure. The image pyramid is a collection of reduced resolution images, which are computed by an iterative procedure [18]. The pyramids can be divided into two categories: the regular pyramids [19] which have some problems [20] due to their fixed decimation process and the irregular pyramids [20] which solve these problems through dynamic graph structures, but their handling is more time consuming due to not specified height of pyramid and size of each level.

Pyramidal models can provide an approach to simulate the mental mechanisms as well as the transformation process from perception to reasoning. This approach can offer sub-optimal algorithms which have the linear computational complexities similar to the mental processes' [21]. Pizlo et al. [22] adopt a multilevel pyramidal model for modeling the size transformation and size perception of human. Haxhimusa et al. [23] applied this approach in order to find near-optimal tour in the traveling salesman problem. They formed a graph where cities were its nodes and the neighboring cities' correlations were its edges. The graph pyramid was built based on the minimum spanning tree principle. The nodes of every level were grouped into trees with a predefined height and applied as the nodes of the next level.

2.3. Graph summarization

Graph summarization methods have a major contribution in resolution reduction of the graphs. The researchers in different disciplines apply different approaches to extract graph summaries. In physics and biology, statistical measures [24] such as degree