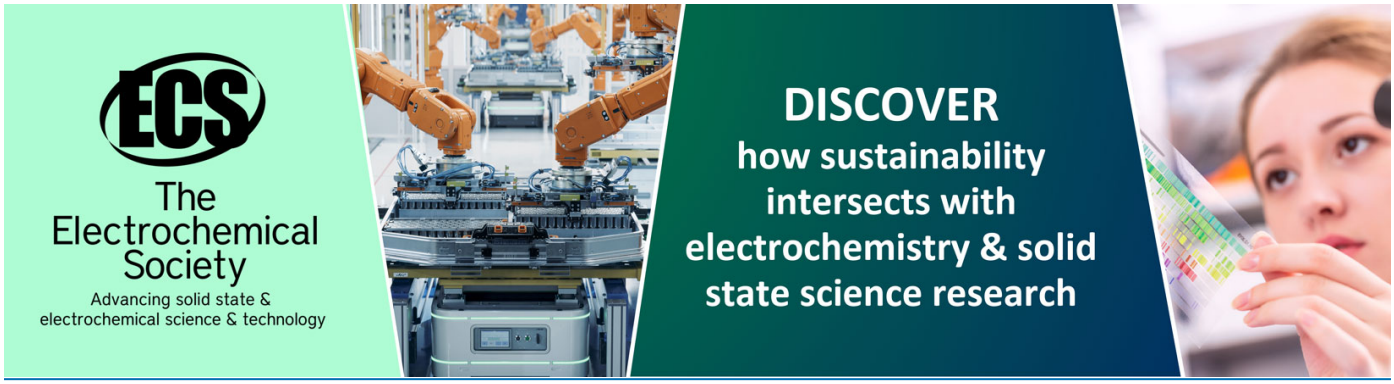
Regular graph construction for semi-supervised learning



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Regular graph construction for semi-supervised learning

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Abstract. Semi-supervised learning (SSL) stands out for using a small amount of labeled points for data clustering and classification. In this scenario graph-based methods allow the analysis of local and global characteristics of the available data by identifying classes or groups regardless data distribution and representing submanifold in Euclidean space. Most of methods used in literature for SSL classification do not worry about graph construction. However, regular graphs can obtain better classification accuracy compared to traditional methods such as k-nearest neighbor (kNN), since kNN benefits the generation of hubs and it is not appropriate for high-dimensionality data. Nevertheless, methods commonly used for generating regular graphs have high computational cost. We tackle this problem introducing an alternative method for generation of regular graphs with better runtime performance compared to methods usually find in the area. Our technique is based on the preferential selection of vertices according some topological measures, like closeness, generating at the end of the process a regular graph. Experiments using the global and local consistency method for label propagation show that our method provides better or equal classification rate in comparison with kNN.

1. Introduction

Semi-supervised learning (SSL) uses large amount of unlabeled data and available labeled data to build classifiers applyied to real problems. As SSL requires less human effort and gives higher accuracy, it is of great interest [10], [2]. Among the current SSL methods, graph based approaches have emerged and highlighted, specially, when no parametric information is available about the data distribution.

Several graph-based methods were developed and much of them are similar to each other. Zhu (2005) [10] arguments that it is more important to construct a good graph than to choose among the methods. However, graph construction is not a well studied area. Only recently, the issue of graph construction has received attention [8], [4], [5].

The most common method used for graph construction is neighbor graphs, for example k-Nearest Neighbors (kNN) graph, where each item is connected to its k nearest neighbors under some distance measure. As kNN method greedily connects the k nearest neighbors to each vertex and may return graphs where some vertices have more than k neighbors, Jebara et al. (2009) [4] proposed the b-matching, which ensures the graph is regular (every vertex with b neighbors) and by experimental results suggest that a regular graph can achieve better classification results compared to kNN. Huang and Jebara (2007) [3] developed an implementation based on belief propagation, but the guaranteed running time of the implementation is $O(bn^3)$. In some cases, like in the work of Ozaki et al. (2011) [6], building a b-matching graph is inviable in terms of computational cost.

In the supervised context, nearest neighbor classification does not work properly in high-dimensional space. Radovanovic et al. (2010) [7] argue that this happen because a hub is an example close to many

other examples in the (high-dimensional) example space. They state that such hubs inherently emerge in high-dimensional data as a side effect of the "curse of dimensionality". Ozaki et al., (2011) [6] extend this argument and made an observation that a hub in the data space also makes a hub in the kNN graph, since kNN graph construction greedily connects a pair of vertices, if the corresponding vertex is among the k closest neighbors of the other example in the original space.

To test this hipotesis, that regular graph can be better for SSL, we introduce a new method for generation of graphs with no hubs. Our method has quadratic time complexity, as kNN algorithm. To evaluate if this technique is better than other that generates hubs, like kNN, we compare the classification accuracy between them using Local and Global Consistency (LGC) algorithm [9] for the label propagation task. The classification results from UCI [1] and Chapelle [2] data sets show the presented method achieves results better or equal than kNN method.

The remainder of this paper is organized as follows. Section 2 defines basic concepts. Section 3 provides the details of the graph construction method introduced and the experimental validation results for the algorithm on benchmark datasets. Concluding remarks are then provided in Section 4.

2. Definitions

Given a set of n examples, $X = \{x_1, \ldots, x_n\}$, semi-supervised classification methods utilize l labeled examples $\{(x1, y1), \ldots, (xl, yl)\}$ and the remaining $u = n - l$ unlabeled examples $\{x_{l+1}, \ldots, x_{l+u}\}$ to infer the missing labels $\{y_{l+1}, \ldots, y_{l+u}\}$ corresponding to the unlabeled examples. For using a graph-based algorithm it is necessary the estimation of a weighted undirected sparse graph G derived from the input data X. In this paper we are interested in how to construct a regular graph from X.

A graph $G = (V, E)$ is formed by a set V of vertices (nodes) and a set E of edges (links) that connect pairs of vertices. The cardinality of V is usually denoted by n, the cardinality of E by m. If two vertices are joined by an edge, they are adjacent and we call them neighbors. Often it is useful to associate numerical values (weights) to the edges or vertices of a graph G. Edge weights can be represented as a function $w : E \to \Re$ that assigns to each edge $e \in E$ a weight $w(e)$. In the context of this work, edge weights describe similarity between the adjacent vertices.

A graph G can be described by the adjacency matrix P, a $N \times N$ square matrix whose entry p_{ij} $(i, j = 1, \ldots, N)$ is equal to 1 when the link p_{ij} exists, and 0 otherwise. The degree d_i of a node i is the number of edges incident with it, and is defined in terms of the adjacency matrix P as $d_i = \sum_{j \in N} p_{ij}$. If a node has a degree much bigger than the others nodes, it is called *hub*. The averaged degree for a network is defined as $\langle d \rangle = \frac{1}{N} \sum_{n \in N} d_n$. Graph-based methods are in general transductive, that means it only works on the labeled and unlabeled training data, and not handle unseen data.

Algorithm 1 Sequencial kNN method

input: data base X, k_{max}
symbols: P - adjacency matrix; R - set of vertices order by a relevance criterium;
G - set of vertices degree initialized as $G : [0, \ldots, 0]_{1 \times N}$

compute kNN $\leftarrow$ getK-NearestNeighbor(X)
compute $R \leftarrow$ getOrderByRelevance(X)
v_i, v_j, $k = 1$
repeat
    $v_i \leftarrow$ getNextNode(R)
    $v_j \leftarrow$ getNearestPossibleNeighbor(v_i, k, k_{max}, kNN)
    if $v_j \neq$ NULL
        connect(P, v_i, v_j, G)
    else
        $k \leftarrow k + 1$
until $\exists\, v_i \mid G(v_i) < k_{max}$
output: P

3. Regular graph construction

We introduce a new method for regular graph construction called *Sequencial kNN* (S-kNN). The method consists in create connections incrementaly, from $k = 1$ to a maximum k_{max} value. In the process a vertex is chosen by a relevance criterium and establish a connection with the disponible nearest neighbor. The relevance criterium order the vertices by a Complex Network measure. Here we use the measure *closeness*: $C_i = \frac{1}{\sum_{x_j \in V} \|x_i - x_j\|}$, where $\| \ . \ \|$ is some distance kernel, and we use Euclidian distance.

Algorithm 1 describes the steps for the graph construction. After computing the k nearest neighbors vector for the vertices and order it by a relevance criterium, we take vertices from the ordered vector and try to connect each vertex to the nearest neighbor into the k_{max} neighbors, that have a degree smaller than k. If it is not possible, we increment k and then, we repeat the process. The algorithm ends when all the vertices have degree bigger or equal than k_{max}. If it does not happen, the vertex that have degree smaller than k_{max} will connect to the k nearest neighbor with smallest degree. The complexity is the same as kNN algorithm.

The experiments were carried out on ten data sets. The first seven are from UCI Machine Learning Repository [1] and the last three are from Chapelle et al. (2006) [2]. For USPS, DIGIT_1 and COil_2 we apply Principal Component Analysis (PCA) to all data sets reducing the dimensions to 50. The matrix was symmetrized as follows $P_{ij} = max(P_{ij}, P_{ji})$. To generate the weighted graph W we use the binary weighting approach, where $W = P$. The labeled points was randomly selected from all the points. The parameter k_{max} was varied from 1 to 20. Averaged classification accuracy of 30 runs is used as the evaluation measure and the results are shown in Table 1.

Table 1. Averaged accuracy with different labeled points.

Data set (# labeled points)	# Instances	# Atributes	# Classes	% Accuracy kNN	% Accuracy S-kNN
Zoo (7)	101	16	7	72.489 ± 11.614	**76.361 ± 9.59**
Zoo (21)				**74.875 ± 5.239**	73.4 ± 4.75
Iris (3)	150	4	3	89.918 ± 4.78	**91.931 ± 4.581**
Iris (9)				89.177 ± 6.732	**90.226 ± 8.048**
Glass (6)	214	9	6	37.115 ± 8.125	**37.894 ± 7.895**
Glass (18)				46.448 ± 6.072	**47.969 ± 7.434**
Breast Cancer(2)	286	9	2	96.279 ± 1.192	**96.755 ± 0.698**
Breast Cancer (6)				91.535 ± 8.336	**94.322 ± 4.51**
Ecoli (8)	336	7	8	**67.903 ± 8.663**	66.283 ± 8.817
Ecoli (24)				76.367 ± 4.835	**76.809 ± 3.706**
Blood transfusion(2)	748	4	2	52.788 ± 14.899	**52.906 ± 17.879**
Blood transfusion (6)				**66.417 ± 8.902**	65.425 ± 11.096
Yeast(10)	1484	8	10	29.398 ± 5.760	**30.474 ± 8.434**
Yeast (30)				41.490 ± 3.762	**41.815 ± 4.310**
USPS (10)	1500	241	2	**83.543 ± 4.596**	82.930 ± 3.356
USPS (100)				**89.609 ± 3.169**	89.516 ± 1.947
DIGIT_1 (10)	1500	241	2	**89.619 ± 7.488**	87.225 ± 7.554
DIGIT_1 (100)				97.033 ± 1.121	**97.307 ± 0.683**
COIL_2(10)	1500	241	2	**65.731 ± 5.19**	**65.738 ± 6.178**
COIL_2(100)				96.938 ± 1.95	**97.297 ± 1.243**

Figure 1 shows the degree distribution for S-kNN and kNN graphs built using the Breast-Cancer data set with $k = 7$. We notice that S-kNN method has almost all vertices with a degree equal 7, less than 250 vertices have degree equal $8, 9, 10$. It generated 2597 edges with the averaged degree equal 7.6. The kNN method has vertices with vary different degree where less than 200 vertices have degree equal 7, the remainig have degree from 8 to 36. It generated 3548 edges with the averaged degree equal 10.4. Figure 2 shows a graph built using the Glass data set with $k = 5$. Bigger the points, bigger the vertice degree. The kNN graph has more bigger points compared to S-kNN.

4. Conclusion

From the experiments results we notice that the introduced method achieves better or equals results than kNN algorithm. This indicates that regular graphs also have good classification accuracy in graph-based

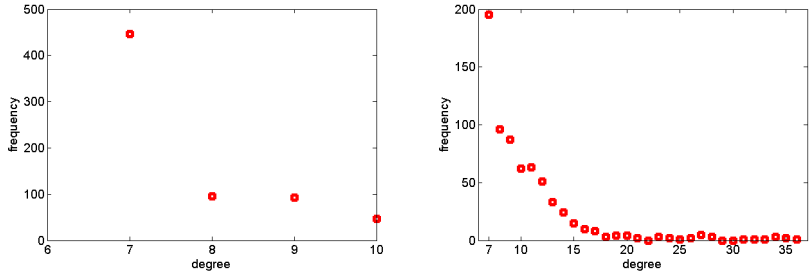

Figure 1. Degree distribution for S-kNN and kNN graphs built using the Breast-Cancer data set, $k = 7$.

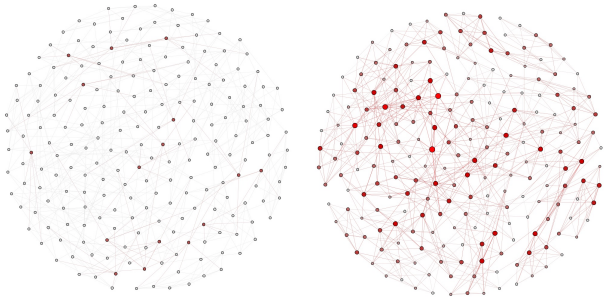

Figure 2. S-kNN and kNN graphs built using the Glass data set, $k = 5$.

SSL. For future work we will do statistic tests to detect if there are differences among algorithms. We also will compare the results to b-matching method and test other measures for the relevance criterium.

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