A One Hour Trip in the World of Graphs, Looking at the Papers of the Last Ten Years

Mario Vento

Dept. of Computer Eng. and Electrical Eng. and
Applied Mathematics University of Salerno
Via Ponte Don Melillo, Fisciano (SA), Italy
mvento@unisa.it

1 Motivations of the Trip

The use of a graph-based pattern representation induces the need to formulate the main operations required in Pattern Recognition in terms of operations on graphs: classification, usually intended as the comparison between an object and a set of prototypes, and learning, which is the process for obtaining a model of a class starting from a set of known samples, are among the key issues that must be addressed using graph-based techniques.

Forty years have passed since the first papers on this topic appear in Pattern Recognition literature: a lot of research effort has been devoted to explore this challenging field and some approaches have been meanwhile consolidated. These notes aren't a scientific paper but some considerations inspiring my future talk at gbr 2013 conference, a little trip in the word of graphs aimed at better knowing treasures and outstanding locations.

2 Trip Diary

The use of graphs in Pattern Recognition dates back to the early seventies, and the paper Thirty years of graph matching in Pattern Recognition" [14] reports a survey of the literature on graph-based techniques since the first years and up to the early 2000's. In the last decade we have assisted to a growing interest in graphs, as confirmed by the number of papers using graphs for different aspects of Pattern Recognition.

We have surely assisted to a maturation of the classical techniques for graph comparison, either exact or inexact; contemporarily we are assisting to a rapid growth of many alternative approaches, such as graph embedding and graph kernels, aimed at making possible the application to graphs of vector-based techniques for classification and learning (such as the ones derived from the statistical classification and learning theory).

The trip is devoted to analyze the main advances registered in graph-based methodologies in the last ten years, looking at the main recent literature on this topic; the aim is to reconstruct an unifying view of these approaches when used in the context of Pattern Recognition tasks.

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The analysis starts from the above mentioned survey [14] and enriches the discussion by considering a selection of the most recent main contributions; consequently, the talk, for the sake of conciseness, will mainly focus on the papers published during the last ten years. At the beginning, the interests of Pattern Recognition researchers on graphs were mainly concentrated on graph matching, either exact or inexact. While for the exact methods the attention was concentrated on the definition of novel algorithms attempting to progressively reduce the computational burden, the approaches used in the inexact methods were inspired to some different rationales:

– Optimal inexact matching algorithms, able to find a solution minimizing the matching cost; it is guaranteed that, if an exact solution exists, it will be found. The algorithms ascribed to this class essentially concentrate on dealing with the input graph variability; the optimality of the solution requires an exploration of the solution space, usually making the algorithms fairly more expensive than the exact ones. Most of the algorithms are based on some forms of Tree search with backtracking, but also other techniques based on group theory or other mathematical properties of the graphs used in the matching process have been proposed.
– Suboptimal or approximate matching algorithms, able to ensure only a local minimum of the matching cost: it is expected that the obtained minimum is close to the global minimum, even if an upper bound of this distance is often unknown, so limiting their applicability to cases in which the maximum error value assumes a secondary importance. The big advantage of this class of algorithms is the polynomial matching time. While tree searching methods of this kind have been developed, the most common approach is based on continuous optimization, by replacing the matching problem, inherently discrete, with a continuous one, usually not linear; the advantage is that it is possible the use of a well established theoretical framework. Another important class of algorithms, although not as common as continuous optimization, is based on the exploitation of the eigenvalues of the adjacency matrix, which are invariant to node permutations, which can help to reduce the computational complexity in the matching process. Also a wide array of other techniques have been used less frequently.
– Error correcting graph matching algorithms, based on the definition of an explicit model of the errors (missing nodes and/or edges, changes on the attributes, etc.); the cheapest sequence of operations needed to transform one graph into the other is used to evaluate a similarity between the two graphs. So, with respect to exact and inexact graph matching, the discussion will be finalized to the presentation of the main advances on these kinds of graph matching algorithms.

Of course what is happening in the recent past, see the journal papers reported in the Section References, cannot be left out of the discussion: in fact, in the last decade we have assisted to the birth and growth of methods facing learning and classification in a rather innovative scientific vision: the computational burden of matching algorithms together with their intrinsic complexity, in opposition to the well established world of statistical Pattern recognition methodologies, suggested new paradigms for the graph-based methods: why don't we try to reduce graph matching and learning to vector-based operations, so as to make it possible the use of statistical approaches?

Two opposite ways of facing the problem, each with its pros and cons: graphs from the beginning to the end", with a few heavy algorithms, but the exploitation of all the information contained into the graphs; on the other side, the risk of loosing discriminating power during the conversion of graphs into vectors (by selecting suitable properties), counterbalanced by the immediate access to all the theoretically assessed achievements of the statistical framework.

These two opposite factions are now simultaneously active, each hoping to overcome the other; ten years ago these innovative methods were in the background, but now they are gaining more and more attention in the scientific literature on graphs.

Graph embedding, intended as the technique that map whole graphs onto points in a vector space, in such a way that similar graphs are mapped onto close points is perhaps the most significant novelty in graph-based in Pattern Recognition in the recent years. Although seminal works on these fields were already present in earlier literature, it is in the last decade that these techniques have gained popularity in the Pattern Recognition community. Bunke et al. [10] present a survey on the topic of graph kernels and graph embeddings, and in [11] extend this review and present these techniques as a way to unify the statistical and structural approaches in Pattern Recognition.

Graph kernels represent a sort of generalization of graph embedding; if we denote with G the space of all the graphs, a graph kernel is a function that maps a couple of graphs onto a real number, and holds similar properties to the dot product defined on vectors. More formally they can be seen as a measure of the similarity between two graphs; however its formal properties allow a kernel to replace the vector dot product in several vector-based algorithms that use this operator (and other functions related to dot product, such as the Euclidean norm). Among the many Pattern Recognition techniques that can be adapted to graphs using kernels we mention Support Vector Machine classifiers and Principal Component Analysis.

Kernels have been used for a long time to extend to the nonlinear case linear algorithms working on vector spaces, thanks to the Mercer's theorem: given a kernel function defined on a compact space X, there is a vector space V and a mapping between X and V such that the value of the kernel computed on two points in X is equal to the dot product of the corresponding points in V. Thus, for compact spaces, a kernel can be seen as an implicit way of performing an embedding into a vector space. Although Mercer's theorem do not apply to graph kernels, in practice these latter can be used as a theoretically sound way to extend a vector algorithm to graphs. Of course, the actual performance of these algorithms strongly depend on the appropriateness (with respect to the task at hand) of the notion of similarity embodied in the graph kernel.

3 Trips Souvenirs

What have we experienced from the trip? The analysis of the recent literature of graph-based techniques shows there is still a warm interest toward the use of this important data structure for facing Pattern Recognition problems. However, a definite interpretation of the best promising future directions seems to be still a bit uncertain: on one hand, we have surely assisted to a maturation of the classical techniques for graph comparison, either exact or inexact; on the other hand, we are assisting to a rapid growth of many alternative approaches, such as graph embedding and graph kernels, whose rationale is to reduce graphs to vectors so as to make it possible the use of the well established statistical theory of classification and learning.

The main questions posed by researchers advocating the graphs from beginning to end" approach could be: Is it really effective to solve a problem starting with graph representations, and going back to vectors, risking to lose important chunks of discriminative power? If so, why don't you renounce to use graphs, and directly use vector-based descriptions from the start?"

The opposite faction could reply: Why do you insist on describing the world by graphs if there is still a lack of completely assessed and computationally acceptable algorithms for classifying and for learning graph prototypes?"

The conclusion? We will discuss!

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