On the use of Factorized Distribution Algorithms for problems defined on graphs

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Abstract

This short paper surveys current work on the use of Factorized Distribution Algorithms for the solution of combinatorial optimization problems defined on graphs. We also advance a number of approaches for future work along this line.

1 Introduction

Population Based Search Methods that use Selection (PBSMS) are non deterministic heuristic search strategies that use a set of points instead of a single one to conduct the search. Genetic Algorithms [1] are one example of PBSMS. They have been applied for the solution of combinatorial optimization problems, including classical problems defined on graphs.

Factorized Distribution Algorithms (FDAs) [3] are another class of PBSMS that combine results from Graphical Models and Evolutionary Computation research, and are considered as a tractable subclass of Estimation Distribution Algorithms [4]. They begin by generating an initial random population of points which are evaluated using the objective function. Some of the points are selected based on their values, and a factorized probabilistic model of their underlying distribution is constructed. This probabilistic model is used to sample the points that will be part of the next population.

The objective of this paper is to make a review of the capabilities of FDAs to deal with problems defined on graphs. The problems under consideration are those where the goal is to find structures (such as Hamiltonian paths, cliques or partitions) on a given simple graph. A necessary condition is that the search for the structures could be transformed in the optimization of a function defined for a set of variables mapping the vertices (or the edges) of the graph.

2 FDAs and their application to graphs problems

FDAs differ in the type of factorization employed and the way this factorization is learned. We describe a number of FDAs that are relevant for our research, a detailed review of FDAs can be found in [2].

The Univariate Marginal Distribution Algorithm (UMDA) [4] is a very simple FDA that generates new solutions by only preserving the proportions of the values of each variable independently of the remaining variables. A Factorized Distribution Algorithm that uses a fixed model of the interaction among variables along the evolution (FDA*) was introduced in [3]. The probabilistic model of the (FDA*) is the so called junction tree, which is a tree whose vertices are subsets of the variables of the problem. The union of all the subsets is the total set of variables. In the tree, the edge between two vertices is labeled with the intersection between these vertices. All vertices between any two pair of vertices A and B contain their intersection. In every generation only a parametric learning of the local joint probabilities of variables in the vertices is done.

While in the (FDA*) the junction tree is built using prior knowledge about the problem and its structure keeps the same along the generations, the Bayesian Optimization Algorithm (BOA) [5] is an example of Bayesian FDAs that learn in every generation a probabilistic model with different structure and represent it using a Bayesian Network (BN). BOA uses a Bayesian metric to measure the goodness of every Bayesian structure found, and a search procedure to search in the space of possible structures. Another class of FDAs is the class of Mixture FDAs. Modeling by finite mixture of distributions concerns modeling a statistical distribution by a mixture (or weighted sum) of other distributions. FDAs that use mixtures of distributions for discrete problems have been proposed in [10,2].

We separate the ways of application of FDAs to problems defined on graphs in two main classes depending on whether the information about the problem structure (e.g. graph topology) is or not used in the construction of the probabilistic model. In the following applications knowledge about the problem structure was not incorporated into the probabilistic model of the FDAs.

In [8] we have employed the Constraint-UMDA (CUMDA) for the search of triangulations on graphs. Although results were encouraging for small graphs, their quality decreased as the number of edges and vertices increase. In the optimization of the triagulation function a set of dependencies among the variables arise that an algorithm that uses the univariate model (e.g. CUMDA) can not capture. In [11] the UMDA and the BOA were used for the problem of hypergraph partitioning. For bisection of regular test graphs the best per-

formance was achieved by BOA. Graph partitioning is also solved in [6] using BOA. In [2] two problems are treated using FDAs: The graph matching is approached using a permutation based representation, and bisection problems are approached using FDAs with mixture distributions. In all of the previous works only small and medium graphs were considered, comparisons with other heuristics different than PBSMS were absent or insufficient.

We present now three main approaches for incorporating information about the graph topology to the probabilistic models in FDAs. The first is the use of the graph to speed the learning of the network structure by Bayesian FDAs. The graph would be used as the starting network of the BN learning algorithm. This approach was proposed in [6], although experiments were not conducted.

The second is to use the graph to construct the junction tree to be used by the FDA*. We have used this approach in [7] for identifying dissections on graphs, and in [9] for the Maximum Satisfiability problem (Max-Sat). Max-Sat is not a graph problem, however a graph representation G' of the interactions between variables can be constructed, and from G' a factorization of the probabilistic model can be built. To find a good factorization starting from G' we have used in [9] an algorithm that extracts a triangulated subgraph of G'. The triangulated subgraph contains a maximum clique of size equal or less than s, where s is a parameter of the algorithm. This heuristic algorithm tries to remove as few edges as possible but guaranteeing that the remaining graph is chordal.

The third approach is the use of Mixture of FDAs. A partition of the initial graph in different subgraphs is done. Every subgraph is triangulated and a junction tree is constructed from it. Each junction tree becomes the skeleton of a different mixture component of the Mixture of FDAs. We have done preliminary experiments with this approach. Compared to the FDA* the approach reduces the number of evaluations, but it is more expensive in terms of the computational time needed to update and sampling the probabilistic model.

3 Conclusions

We have presented different ways to use FDAs for problems defined on graphs. However one important question is still open: Can FDAs be more efficient than other heuristics for problems defined on graphs? Probably the answer is not categorical, and there is a niche of problems where FDAs can be superior. Further research is needed to know which are the limits of FDAs and how can they be improved. The approaches we have presented in this paper show different ways of orienting the search in this direction.

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