# On the performance of a cavity method based algorithm for the Prize-Collecting Steiner Tree Problem on graphs

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(Dated:)

# Abstract

We study the behavior of an algorithm derived from the cavity method for the Prize-Collecting Steiner Tree (PCST) problem on graphs. The algorithm is based on the zero temperature limit of the cavity equations and as such is formally simple (a fixed point equation resolved by iteration) and distributed (parallelizable). We provide a detailed comparison with state-of-the-art algorithms on a wide range of existing benchmarks networks and random graphs. Specifically, we consider an enhanced derivative of the Goemans-Williamson heuristics and the DHEA solver, a Branch and Cut Linear/Integer Programming based approach. The comparison shows that the cavity algorithm outperforms the two algorithms in most large instances both in running time and quality of the solution. Finally we prove a few optimality properties of the solutions provided by our algorithm, including optimality under the two post-processing procedures defined in the Goemans-Williamson derivative and global optimality in some limit cases.

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#### I. INTRODUCTION

The cavity method developed for the study of disordered systems in statistical physics has led in the recent years to the design of a family of algorithmic techniques for combinatorial optimization known as message-passing algorithms (MPA). In spite of the numerical evidence of great potentialities of these techniques in terms of efficiency and quality of results for many optimization problems, their use in real-world problems has still to be fully expressed. The main reasons for this reside in the fact that the derivation of the equations underlying the algorithms are in many cases non-trivial and that the rigorous and numerical analyses of the cavity equations are still largely incomplete. Both rigorous results and benchmarking would play an important role in helping the process of integrating MPAs with the existing techniques.

In what follows we focus on a very well known NP-hard optimization problem over networks, the so-called Prize Collecting Steiner Tree problem on graphs (PCST). The PCST problem can be stated in general terms as the problem of finding a connected subgraph of minimum cost. It has applications in many areas ranging from biology, e.g. finding protein associations in cell signaling [1, 2], to network technologies, e.g. finding optimal ways to deploy fiber optic and heating networks for households and industries [3].

Though the cavity equations have been developed for the study of mean field models for disordered systems, the range of their applicability is known to go beyond these problems.

In this paper we show how MSGSTEINER – an algorithm derived from the zero temperature cavity equations [2] – compares with state-of-the-art techniques on benchmarks problem instances. Specifically, we provide comparison results with an enhanced derivative of the Goemans-Williamson heuristics (MGW) [4, 5] and with the DHEA solver [6], a Branch and Cut Linear/Integer Programming based approach. We made the comparison both on random networks and in known benchmarks. We show that MSGSTEINER typically outperforms the state-of-the-art algorithms in the largest instances of the PCST problem both in the values of the optimum and in running time.

Finally, we show how some aspects of the solutions can be provably characterized. Specifically we show some optimality properties of the fixed points of the cavity equations, including optimality under the two post-processing procedures defined in MGW (namely *Strong Pruning* and *Minimum Spanning Tree*) and global optimality of the MPA solution in some limit

cases.

#### A. Related work

The method and the algorithm described here are a generalization of the technique presented in ref. [7]. In [7] the algorithm is tested on different families of random graphs for the more specific case of bounded depth (D) Steiner tree problem, which can be recovered from the PCST problem by sending to infinity the weights of the so-called terminal nodes. In the cases of Erdos-Renyi random graphs and for scale-free graphs the numerical performance of the algorithm have been shown to be extremely good though there exits no rigorous results to compare with. Interestingly enough the case of complete graphs with random weights allows for a comparison with rigorous asymptotic results. The scaling coefficients of the power law for the average minimum cost and number of Steiner nodes as a function of the size N of the graph was calculated exactly in ref. [8], where it was also rigorously established that the critical depth for the bounded-depth Minimum Spanning Tree and Steiner Tree on random complete graphs is  $D = \log_2 \log N$ . Extensive numerical studies up top  $N = 10^5$ which for brevity we do not report in detail, show that the cavity approach provides solutions which have a minimum cost that is below that of the greedy algorithm analyzed in [8] and that there is slow convergence to the exact scaling parameters. This fact corroborates the conjecture that the cavity approach could be asymptotically exact and reproduce the results of [8]. While this is not totally unexpected for statistical physics of random systems (the cavity approach is known to be very accurate on mean-field problems defined over complete graphs), it is important for the rigorous foundation of the cavity method itself. There exist in fact very few model problems on which the zero temperature cavity approach can be proven to be exact, one famous example being the matching problem [9]. NP-complete problems (considered in their typical realizations) are particularly elusive in this respect, possibly due to the local nature of the cavity algorithms. Therefore, having at hand a nontrivial problem which can be analyzed rigorously as in [8] constitutes an interesting case also for the rigorous understanding of the cavity method.

#### II. THE PROBLEM: PRIZE COLLECTING STEINER TREES

In the following we will describe the Prize-Collecting Steiner Tree problem on Graphs (see e.g. [5, 10]).

**Definition 1.** Given a network G = (V, E) with positive (real) weights  $\{c_e : e \in E\}$  on edges and  $\{b_i : i \in V\}$  on vertices, consider the problem of finding the connected subgraph G' = (V', E') that minimizes  $H(V', E') = \sum_{e \in E'} c_e - \lambda \sum_{i \in V'} b_i$ , i.e. to compute the minimum:

$$\min_{E' \subseteq E, V' \subseteq V} \sum_{e \in E'} c_e - \lambda \sum_{i \in V'} b_i. \tag{1}$$

$$(V', E') \text{ connected}$$

It can be easily seen that a minimizing sub-graph must be a tree (links closing cycles can be removed, lowering H). The parameter  $\lambda$  regulates the tradeoff between the edge costs and vertices prizes, and its value has the effect to determine the size of the subgraph G': for  $\lambda = 0$  the empty subgraph is optimal, whereas for  $\lambda$  large enough the optimal subgraph includes all nodes.

This problem is known to be NP-hard, implying that no polynomial algorithm exists that can solve any instance of the problem unless NP = P. To solve it we will use a variation of a very efficient heuristics based on belief propagation developed on [7] that is known to be exact on some limit cases [7, 11]. We will partially extend the results in [11] to a more general PCST setting.

# A. Rooted, depth bounded PCST and forests

We will deal with a variant of the PCST called D-bounded rooted PCST (D-PCST). This problem is defined by a graph G, an edge cost matrix c and prize vector b along with a selected "root" node r. The goal is to find the r-rooted tree with maximum depth D of minimum cost, where the cost is defined as in (1). A general PCST can be reduced to D-bounded rooted PCST by setting D = |V| and probing with all possible rootings, slowing the computation by a factor |V| (we will see later a more efficient way of doing it). A second variant which we will consider is the so-called R multi-rooted D-bounded Prize Collecting Steiner Forest ((R, D)-PCSF). It consists of is a natural generalization of the

previous problem: a subset R of "root" vertices is selected, and the scope is to find a forest of trees of minimum cost, each one rooted in one of the preselected root nodes in R.

#### B. Local constraints

The cavity formalism can be adopted and made efficient if the global constraints which may be present in the problem can be written in terms of local constraints. In the PCST case the global constraint is connectivity which can be made local as follows.

We start with the graph G=(V,E) and a selected root node  $r \in V$ . To each vertex  $i \in V$  there is an associated couple of variables  $(p_i,d_i)$  where  $p_i \in \partial i \cup \{*\}$ ,  $\partial i = \{j:(ij) \in E\}$  denotes the set of neighbors of i in G and  $d_i \in \{1,\ldots,D\}$ . Variable  $p_i$  has the meaning of the parent of i in the tree (the special value  $p_i = *$  means that  $i \notin V'$ ), and  $d_i$  is the auxiliary variable describing its distance to the root node (i.e. the depth of i). To correctly describe a tree, variables  $p_i$  and  $d_i$  should satisfy a number of constrains, ensuring that depth decreases along the tree in direction to the root, i.e.  $p_i = j \Rightarrow d_i = d_j + 1$ . Additionally, nodes that do not participate to the tree  $(p_i = *)$  should not be parent of some other node, i.e.  $p_i = j \Rightarrow p_j \neq *$ . Note that even though  $d_i$  variables are redundant (in the sense that they can be easily computed from  $p_j$  ones), they are crucial to maintain the locality of the constraints. For every ordered couple i,j such that  $(ij) \in E$ , we define  $f_{ij}(p_i,d_i,p_j,d_j) = \mathbb{1}_{p_i=j\Rightarrow d_i=d_j+1\land p_j\neq *} = 1 - \delta_{p_i,j}\left(1-\delta_{d_i,d_j+1}(1-\delta_{p_j,*})\right)$  (here  $\delta$  is the Kroenecker delta). The condition of the subgraph to be a tree can be ensured by imposing that  $g_{ij} = f_{ij}f_{ji}$  has to be equal to one for each edge  $(ij) \in E$ . If we extend the definition of  $c_{ij}$  by  $c_{i*} = \lambda b_i$ , then (except for an irrelevant constant additive term), the minimum in (1) equals to:

$$\min \{ \mathcal{H}(\mathbf{p}) : (\mathbf{d}, \mathbf{p}) \in \mathcal{T} \}, \tag{2}$$

where  $\mathbf{d} = \{d_i\}_{i \in V}, \ \mathbf{p} = \{p_i\}_{i \in V}, \ \mathcal{T} = \{(\mathbf{d}, \mathbf{p}) : g_{ij}(p_i, d_i, p_j, d_j) = 1 \ \forall (ij) \in E\}$  and

$$\mathcal{H}(\mathbf{p}) \equiv \sum_{i \in V} c_{ip_i}.$$
 (3)

This new expression for the energy accounts for the sum of taken edge costs plus the sum of uncollected prizes and has the advantage of being non-negative.

#### III. DERIVATION OF THE MESSAGE-PASSING CAVITY EQUATIONS

The algorithmic scheme we propose originates from the cavity method of statistical physics, a technique which is known in other fields under different names, namely Cavity equations, Belief Propagation (BP), Max-Sum or Sum-Product equations (MS). From a numerical point of view, message-passing algorithms are distributed algorithm which allow for a very fast resolution of inference and optimization problems [12], even for large networks. A recent review can be found in [13]. The starting point for the equations is the Boltzmann-Gibbs distribution:

$$P(\mathbf{d}, \mathbf{p}) = \frac{\exp(-\beta \mathcal{H}(\mathbf{p}))}{Z_{\beta}},\tag{4}$$

where  $(\mathbf{d}, \mathbf{p}) \in \mathcal{T}$ ,  $\beta$  is a positive parameter (called inverse temperature), and  $Z_{\beta}$  is a normalization constant (called partition function). In the limit  $\beta \to \infty$  this probability concentrates on the configurations which minimize  $\mathcal{H}$ . The BP approximation consists in a weak correlation assumption between certain probability distributions of single  $(p_i, d_i)$  pairs called "cavity marginals". Given  $i, j \in V$ , the cavity marginal  $P_{ji}(d_j, p_j)$  is defined as the marginal distribution  $\sum_{(d_k, p_k)_{k \in V \setminus \{j, i\}}} P_{G^{(i)}}(\mathbf{d}, \mathbf{p})$  on a graph  $G^{(i)}$  from which node i has been temporally removed. The BP equations are derived by assuming that the cavity marginals are uncorrelated and as such satisfy the following closed set of equations (see e.g. [13] for a general discussion):

$$P_{ji}(d_j, p_j) \propto e^{-\beta c_{jp_j}} \prod_{k \in \partial j \setminus i} Q_{kj}(d_j, p_j)$$
(5)

$$Q_{kj}(d_j, p_j) \propto \sum_{d_k} \sum_{p_k} P_{kj}(d_k, p_k) g_{jk}(d_k, p_k, d_j, p_j).$$
 (6)

This assumption is correct if G is a tree, in which case (5)-(6) are exact and have a unique solution. Equations (5)-(6) can be seen as fixed point equations, and solutions are normally searched through iteration: substituting (6) onto 5 and giving a time index t + 1 and t to the cavity marginals in respectively the left and right hand side of the resulting equation, this system is iterated until numerical convergence is reached. Cavity marginals are often called "messages" because they can be thought of as bits of information that flow between edges of the graph during time in this iteration. On a fixed point, the BP approximation to

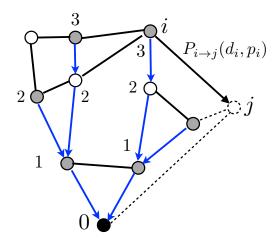


Figure 1. A schematic representation of the Prize Collecting Steiner Tree problem and its local representation. Numbers next to the nodes are the distances (depths) from the root node (black node). The prize value is proportional to the darkness of the nodes. Arrows are the pointers from node to node. Distances and pointers are used to define the connectivity constraints which appear in the message-passing equations.— Blue arrows represent a potential solution.

the marginal is computed as

$$P_{j}(d_{j}, p_{j}) \propto e^{-\beta c_{j} p_{j}} \prod_{k \in \partial j} Q_{kj}(d_{j}, p_{j}).$$

$$(7)$$

# Max-sum: $\beta \to \infty$ limit

In order to take the  $\beta \to \infty$  limit, (6) can be rewritten in terms of "cavity fields"

$$\psi_{ii}\left(d_{i}, p_{i}\right) = \beta^{-1} \log P_{ii}\left(d_{i}, p_{i}\right) \tag{8}$$

$$\phi_{kj}(d_j, p_j) = \beta^{-1} \log Q_{kj}(d_j, p_j).$$
 (9)

The BP equations take the so-called MS form:

$$\psi_{ji}(d_{j}, p_{j}) = -c_{jp_{j}} + \sum_{k \in \partial j \setminus i} \phi_{kj}(d_{j}, p_{j}) + C_{ji}$$

$$\phi_{kj}(d_{j}, p_{j}) = \max_{p_{k}, d_{k}: g_{jk}(d_{k}, p_{k}, d_{j}, p_{j}) = 1} \psi_{kj}(d_{k}, p_{k}),$$
(11)

$$\phi_{kj}(d_j, p_j) = \max_{p_k, d_k: g_{jk}(d_k, p_k, d_j, p_j) = 1} \psi_{kj}(d_k, p_k),$$
(11)

where  $C_{ji}$  is an additive constant chosen to ensure  $\max_{d_j,p_j} \psi_{ji}(d_j,p_j) = 0$ 

Computing the right side of (11) is in general too costly in computational terms. Fortunately, the computation can be carried out efficiently by breaking up the set over which the max is computed into smaller (possibly overlapping) subsets. We define

$$A_{kj}^{d} = \max_{p_{k} \neq j,*} \psi_{kj}(d, p_{k}) \tag{12}$$

$$B_{kj}^{d} = \psi_{kj}\left(d, *\right) \tag{13}$$

$$C_{kj}^{d} = \psi_{kj}\left(d, j\right). \tag{14}$$

Equation (11) can now be rewritten as:

$$A_{ji}^{d} = \sum_{k \in \partial i \setminus i} E_{kj}^{d} + \max_{k \in \partial i \setminus j} \left\{ -c_{jk} - E_{kj}^{d} + A_{kj}^{d-1} \right\}$$
 (15)

$$B_{ji} = -c_{j*} + \sum_{k \in \partial j \setminus i} D_{kj} \tag{16}$$

$$C_{ji}^d = -c_{ji} + \sum_{k \in \partial j \setminus i} E_{kj}^d \tag{17}$$

$$D_{ji} = \max\left(\max_{d} A_{ji}^{d}, B_{ji}\right) \tag{18}$$

$$E_{ji}^{d} = \max\left(C_{ji}^{d+1}, D_{ji}\right). \tag{19}$$

Using some simple efficiency tricks including computing  $\sum_{k\in\partial j\setminus i} E^d_{kj}$  as  $\sum_{k\in\partial j} E^d_{kj} - E^d_{ki}$ , the computation of the right side of (15)-(19) for all  $i\in\partial j$  can be done in a time proportional to  $D|\partial j|$ , where D is the depth bound. The overall computation time is then O(|E|D) per iteration.

## B. Total fields

In order to identify the minimum cost configurations, we need to compute the total marginals, i.e. the marginals in the case in which no node has been removed from the graph. Given cavity fields, the total fields  $\psi_j(d_j, p_j) = \lim_{\beta \to \infty} \beta^{-1} \log P_j(d_j, p_j)$  can be written as:

$$\psi_{j}(d_{j}, p_{j}) = -c_{jp_{j}} + \sum_{k \in \partial j} \phi_{kj}(d_{j}, p_{j}) + C_{j},$$
(20)

where  $C_j$  is again an additive constant that ensures  $\max_{d_j,p_j} \psi_j (d_j, p_j) = 0$ . In terms of the above quantities we find  $\psi_j (d_j, i) = F_{ji}^d \stackrel{def}{=} \sum_{k \in \partial j} E_{kj}^d + \left(-c_{ij} - E_{ji}^d + A_{ji}^{d-1}\right)$  if  $i \in \partial j$  and  $\psi_j (d_j, *) = G_j \stackrel{def}{=} -c_{j*} + \sum_{k \in \partial j} D_{kj}$ . The total fields can be interpreted as (the Max-Sum approximation to) the relative negative energy loss of chosing a given configuration for variables  $p_j, d_j$  instead of their optimal choice, i.e.  $\psi_j (d_j, p_j) = \min \{\mathcal{H}(\mathbf{p}') : (\mathbf{d}', \mathbf{p}') \in \mathcal{T}\} - \min \{\mathcal{H}(\mathbf{p}') : (\mathbf{d}', \mathbf{p}') \in \mathcal{T}, d_j = d'_j, p_j = p'_j\}$ . In particular, in absence of degeneracy, the maximum of the field is attained for values of  $p_j, d_j$  corresponding to the optimal energy.

# C. Iterative dynamics and reinforcement

Equations (15)-(19) can be thought as a fixed-point equation in a high dimensional euclidean space. This equation could be solved by repeated iteration of the quantities A, B, and C starting from an arbitrary initial condition, simply by adding an index (t + 1) to A, B, C in the left-hand side of (11) and index (t) to all other instances of A, B, C, D, E.

This system converges in many cases. When it does not converge, a technique called reinforcement is of help [14]. The idea is to perturbate the right side of (10) and (20) by adding the term  $\gamma_t \psi_j^t(d_j, p_j)$  for a (generally small) scalar factor  $\gamma_t$ . The resulting equations become:

$$A_{ji}^{d}\left(t+1\right) = \sum_{k \in \partial j \setminus i} E_{kj}^{d}\left(t\right) + \tag{21}$$

$$+ \max_{k \in \partial j \setminus i} \left\{ -c_{jk} - E_{kj}^{d}(t) + A_{kj}^{d-1}(t) + \gamma_t F_{jk}^{d}(t) \right\}$$
 (22)

$$B_{ji}(t+1) = -c_{j*} + \sum_{k \in \partial j \setminus i} D_{kj}(t) + \gamma_t G_j(t)$$
(23)

$$C_{ji}^{d}(t+1) = -c_{ji} + \sum_{k \in \partial j \setminus i} E_{kj}^{d}(t) + \gamma_{t} F_{ji}^{d}(t)$$
(24)

$$D_{ji}(t) = \max \left\{ \max_{d} A_{ji}^{d}(t), B_{ji}(t) \right\}$$

$$(25)$$

$$E_{ji}^{d}(t) = \max \left\{ C_{ji}^{d+1}(t), D_{ji}(t) \right\}$$
(26)

$$G_{j}(t+1) = -c_{j*} + \sum_{k \in \partial j} D_{kj}(t) + \gamma_{t} G_{j}(t)$$
 (27)

$$F_{ji}^{d}(t+1) = \sum_{k \in \partial j} E_{kj}^{d}(t) + \left(-c_{ji} - E_{ij}^{d}(t) + A_{ij}^{d-1}(t)\right) +$$
(28)

$$+\gamma_t F_{ji}^d(t). (29)$$

In our experiments, the equations converge for a sufficiently large  $\gamma_t$ . The strategy we adopted is, when the equations do not converge, to start with  $\gamma_t = 0$  and slowly increase it until convergence in a linear regime  $\gamma_t = t\rho$  (although other regimes are possible). The number of iterations is then found to be inversely dependent on the parameter  $\rho$ . This strategy could be interpreted as using time-averages of the MS marginals when the equations do not converge to gradually bootstrap the system into an (easier to solve) system with sufficiently large external fields. A C++ implementation of these equations can be found

(in source form) on [15]. Note that the cost matrix  $(c_{ij})$  need not to be symmetric, and the same scheme could be used for directed graphs (using  $c_{ji} = \infty$  if  $(i, j) \in E$  but  $(j, i) \notin E$ ).

# D. Root choice

The PCST formulation given in the introduction is unrooted. The MS equations on the other hand, need a predefined root. One way of reducing the unrooted problem to a rooted problem is to solve N = |V| different problems with all possible different rooting, and choose the one of minimum cost. This unfortunately adds a factor N to the time complexity. Note that in the particular case in which some vertex has a large enough prize to be necessarily included in an optimal solution (e.g.  $\lambda b_i > \sum_{e \in E} c_e$ ), this node can simply be chosen as as root.

We have devised a more efficient method for choosing the root in the general case, which we will now describe. Add an extra new node r to the graph, connected to every other node with identical edge cost  $\mu$ . If  $\mu$  is sufficiently large, the best energy solution is the (trivial) tree consisting in just the node r. Fortunately, a solution of the MS equations on this graph gives additional information: for each node j in the original graph, the marginal field  $\psi_j$  gives the relative energy shift of selecting a given parent (and then adjusting all other variables in the best possible configuration). Now for each j, consider the positive real value  $\alpha_j = -\psi_j(1,r)$ , that corresponds with the best attainable energy, constrained to the condition that r is the parent of j. If  $\mu$  is large enough, this energy is the energy of a tree in which only j (and no other node) is connected to r (as each of these connections costs  $\mu$ ). But these trees are in one to one correspondence with trees rooted at j in the original graph. The smallest  $\alpha_j$  will thus identify an optimal rooting.

Unfortunately the information carried by these fields is not sufficient to build the optimal tree. Therefore one needs to select the best root j and run the MS equations a second time on the original graph using this choice.

#### E. Comparision with other techniques

We compared the performance of MSGSTEINER with the three different algorithms: two that employ an integer linear programming strategy to find an optimal subtree, namely the Lagrangian Non Delayed Relax and Cut (LNDRC) [16] and branch-and-cut (DHEA) [6], and modified version of the Goemans and Williamson algorithm (MGW)[5].

#### 1. Integer Linear programming

The goal of the Integer linear programming (ILP) is to find an integer solution vector  $x^* \in \mathbb{Z}^n$  such that:

$$c^T x^* = \min\{c^T x^* \mid Ax \ge b, \ x \in \mathbb{Z}^n\},$$
 (30)

where a matrix  $A \in \mathbb{R}^{m*n}$  and vector  $b \in \mathbb{R}^m$  and  $c \in \mathbb{R}^n$  are given. Many graph problems can be formulated as an integer linear programming problem [17]. In general, solving (30) with  $x^* \in \mathbb{Z}$  is NP-Complete. The standard approach consists in solving (30) for  $x^* \in \mathbb{R}$  (a relaxation of the original problem) and use the solution as a guide for some heuristics or complete algorithm for the integer case. The relaxed problem can be solved by many classical algorithms, like the Simplex Method [18] or Interior Point methods. In order to map the PCST problem in a ILP problem we introduce a variable vector  $z \in \{0, 1\}^E$  and  $y \in \{0, 1\}^V$  where the component for an edge in E or for a vertex in V is one if and only if it is included in the solution, zero otherwise. Now (1) can be written as

$$H = \sum_{e \in E} c_e z_e - \sum_{i \in V} b_i y_i , \qquad (31)$$

and the constraints  $Ax \geq b$  in (30) generally involve all the variable z and y and describe the problem. For the PCST, and in general for hard problems, the number of constraints grows exponentially with the problem size[17]. DHEA and LNRDC use different techniques to tackle the problems of enormous number of constraints. Both programs are able in principle to prove the optimality of solution, and when is not the case they are able to give a lower bound for the value of the optimum.

#### 2. Goemans-Williamson

The MGW algorithm is based on the primal-dual method for approximation algorithms [4]. The starting point is still the ILP formulation of the problem (30), but it employs a controlled approximation scheme that enforces the cost of any solution to be at most twice as large as the optimum one. In addition, MGW implements two different post-processing

strategies, namely a pruning scheme that is able to eliminate some nodes while lowering the cost, and the computation of the minimum spanning tree in order to find an optimal rewiring of the same set of nodes. The overall running time is  $\mathcal{O}(n^2 \log n)$ . A complete description is available in [4].

#### IV. COMPUTATIONAL EXPERIMENTS

#### A. Instances

Experiments were performed on several classes of instances:

- C, D and E available at [19] and derived from the Steiner problem instances of the OR-Library [20]. This set of 120 instances was previously used as benchmark for algorithms for the PCST[20]. The solutions of these instances were obtained with the algorithms[6, 16]. The class C, D, E have respectively 500, 1000, 2000 node and are generated at random, with average vertex degree is either 2.5, 4, 10 or 50. Every edge cost is a random integer in the interval [1, 10]. There are either 5, 10, n/6, n/4 or n/2 vertices with prizes different from zero and random integer generated in the interval [1, maxprize] where maxprize is either 10 or 100. Thus, each of the classes C, D, E consists of 40 graphs.
- K and P available at [19]. These instances are provided in [5]. In the first group instances are unstructured. The second group includes random geometric instances designed to have a structure somewhat similar to street maps. Also the solution of these instances were found with the algorithms [6, 16].
- H are the so-called hypercubes instances proposed in [21]. Sets of artificially generated and very difficult instances for the Steiner tree problem. Graphs are d-dimensional hypercubes with  $d \in 6, ..., 12$ . For each value of d, the corresponding graph has  $2^d$  vertices and  $d \cdot 2^{d-1}$  edges. We used the prized version of these instances defined in [6]. For almost all instances in this class the optimum is unknown.
- i640 are the so-called incidence instances proposed in [22] for the Minimum Steiner Tree problem. These instances have 640 nodes and only the nodes in a subset  $K \subseteq V$

have prizes different from zero (in the original problem these were terminals). The weight on each edge (i, j) is defined with a sample r from a normal distribution, rounded to an integer value with a minimum outcome of 1 and maximum outcome of 500, i.e.,  $c_{ij} = \min\{\max\{1, round(r)\}, 500\}$ . However, to obtain a graph that is much harder to reduce by preprocessing techniques three distributions with a different mean value are used. Any edge (i, j) is incident to none, to one, or to two vertices in subset K. The mean of r is 100 for edges (i, j) with  $i, j \notin K$ , 200 on edges with one end vertex in K, and 300 on edges with both ends in K. Standard deviation for each of the three normal distributions is 5. In order to have prizes also on vertices we extracted uniformly from all integer in the interval between 0 and  $4 * max_{edge}$  where  $max_{edge}$  is the maximum value of edges in the samples considered. There are 20 variants combining four different number of vertices in K (rounding to the integer value [.]):  $|k| = [\log_2 |V|]$ ,  $[\sqrt{V}]$ ,  $[\sqrt{V}]$ ,  $[2\sqrt{V}]$ , and [|V|/4] with five edge number: |E| = [3|V|/2], 2|V|,  $[|V|\log |V|]$ ,  $[2V|\log |V|]$ , and [|V|/(|V|-1)/4]. Each variant is drawn five times, giving 100 instances.

• Class R. The last class of samples are G(n,p) random graphs with n vertices and independent edge probability p = (2ν)/(n-1). The parameter ν is the average node degree, that was chosen as ν = 8. The weight on each edge (i, j) can take three different value, 1, 2 and 4, with equal probability ½. Node prizes were extracted uniformly in the interval [0, 1]. We generated different graphs with four different values of λ (λ = 1.2, 1.5, 2 or 3), see (1), in order to explore different regimes of solution sizes. We find that the average number of nodes that belong to the solution for λ = 1.2, 1.5, 2 and 3 are respectively about 14%, 33%, 51%, 67% of the total nodes in the graph. We have created twelve instances of different size for the four class of random graph, from n = 200 up to n = 4000 nodes. For each parameter set we generated ten different realizations. The total number of samples is 480.

The MSGSTEINER algorithm was implemented in C++ and run on a single core of an AMD Opteron Processor 6172, 2.1GHz, 8 Gb of RAM, with Linux, g++ compiler, -O3 flag activated. A C++ implementation of these equations can be found in source form on [15]. The executable of DHEA is available in [19], and in order to compare the running time we ran DHEA and MSGSTEINER on the same workstation. The executable of LNDRC and

MGW programs was not available. We implemented the non-rooted version of MGW to compare only the optimum on the random graph instances.

# B. Results

We analyzed two numeric quantities: the time to find the solution, and the gap between the cost of the solution and the best known lower bound (or the optimum solution when available) typically found with programs based on linear programming. The gap is defined as  $gap = 100 \cdot \frac{Cost-LowerBound}{lowerBound}$ .

In Table (I) we show the comparison between MSGSTEINER and the DHEA program. DHEA is able to solve exactly K, P and C, D, E instances. The worst performance of MSGSTEINER is on the K class, where the average gap is about 2.5%. In this class the average solution is very small as it comprises only about 4.4% of total nodes of the graph. MSGSTEINER seems to have most difficulty with small subgraphs. MSGSTEINER is able to find solutions very close to the optimum for the P class, that should be model a street network. MSGSTEINER is also able to find solutions very close to the optimum, with a gap inferior to 0.025% on the C, D, and E classes.

In Figure (2) we show the gap of MSGSTEINER and MGW from the optimum values found by the DHEA program in the class R. MSGSTEINER gaps are almost negligible (always under 0.05%) and tend to zero when the size grows. MGW gaps instead are always over 1%. For intermediate size of solutions trees the gaps of MGW are over 3%.

In Figure (3) we show the running time for the class R, with increasing solution tree size. In general we observe that the running time of MSGSTEINER grows much slower than the one of DHEA for increasing number of nodes in the graph and MSGSTEINER largely outperforms DHEA in computation time for large instances; furthermore the differences between the algorithms became specially and large for large expected tree solution. In at least one case DHEA could not find the optimum solution whithin the required maximum time and the MSGSTEINER solution was slightly better.

The class i640 consists in graphs with varying number of edges and nodes, and a varying number of nodes with non-zero prize. We define K as the subset of nodes with non-zero prize. Table (II) shows, for each type of graph, the average time and the average gap on five different realizations of the graphs for MSGSTEINER and DHEA algorithms. We set

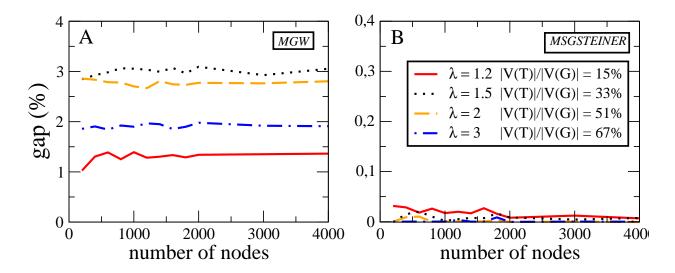


Figure 2. Plot of the Gap of the MSGSTEINER and MGW from the optimum found by DHEA program. MSGSTEINER gaps are always under 0.05%. MGW gaps are always over 1% and for intermediate sizes of the solution tree the gaps of MGW are over 3%.

the time limit to find a solution of DHEA to 2000 seconds. We observe that DHEA obtains good performance in terms of the optimality of the solution when the size of subset K is small. MSGSTEINER finds better result than DHEA when the size of K is sufficiently large, within a time of one or two order of magnitude smaller. Moreover DHEA seems to have difficulty to find reasonable good solution when the graph have high connectivity.

We show in Table (III) a comparison between MSGSTEINER, LNDRC [16] and DHEA. The results and running time of LNDRC are taken from [16]. The computer reportedly used for the optimization is comparable with ours. We have imposed to DHEA a time limit of 6000 seconds and we show two results of MSGSTEINER with different values of the reinforcement parameter. The lower bound is taken from [16]. In almost all instance MSGSTEINER obtains better results, both in time and in quality of solution. The difference is accentuated for large instances. As expected, decreasing the reinforcement parameter allows to find lower costs at the expense of larger computation times.

#### V. POST-PROCESSING AND OPTIMALITY

For this section we will assume unbounded depth D. Results are not easily generalizable to the bounded-D case. Results in this section apply to the non-reinforced MS equations

Group	MS gap	MS time (s)	DHEA gap	DHEA time	(s) Size Sol
K	2.62%	6.51	0.0%	127.97	4.4%
P	0.46%	2.31	0.0%	0.18	31.4%
$\mathbf{C}$	0.006%	16.24	0.0%	2.30	20.2%
D	0.005%	35.06	0.0%	16.12	20.2%
E	0.024%	305.49	0.0%	1296.11	26.4%

Table I. Results class KPCDE

Name	time MS	time DHEA	gap MS (%)	gap DHEA (%)
0-0	0.8	0.2	1.3	0
0-1	2.5	4.2	1.0	0
0-2	100.8	226.6	1.4	0
0-3	1.2	0.3	0.05	0
0-4	37.3	72.8	1.8	0
1-0	1.0	0.85	0.3	0
1-1	2.6	1060.1	1.2	1.5
1-2	90.6	1133.8	0.7	0.2
1-3	1.5	3.8	0.8	0
1-4	33.7	2000.0	1.8	7.8
2-0	0.8	0.7	0.1	0
2-1	4.3	2000.0	2.2	11.6
2-2	149.7	2011.1	0.8	14.8
2-3	1.2	12.0	0.2	0
2-4	39.2	2001.0	1.9	11.2
3-0	1.1	2.4	0.3	0
3-1	3.9	2001.0	1.7	5.6
3-2	112.6	2015.1	0.8	4.9
3-3	1.6	145.3	0.2	0
3-4	33.1	2000.5	1.2	59.9
mean	31.0	834.6	1.0	5.9

Table II. Results i640 class

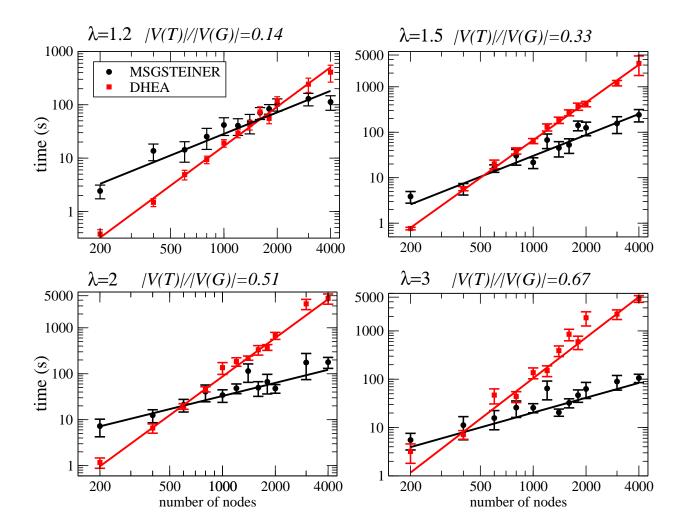


Figure 3. Result on the random graphs class R. Points correspond to the running time of MSG-STEINER and DHEA versus graph size. The four cases show how running time behavior depends on size of the expected solution tree. The quantities shown in figure are averaged over ten different realizations. Data are fitted with function  $y = ax^b$ . The b values found for DHEA are respectively (clockwise from top-left): 2.4, 2.8, 2.8, 2.8. BP performance is as expected roughly linear in the number of vertices. The fitted b parameters are (clockwise from top-left): 1.5, 1.3, 1, 1. For instances that are large enough, the running time of MSGSTEINER is smaller than the one of DHEA and the difference increases with the expected solution tree.

( $\gamma_t = 0$ ). The results here are based in construction of certain trees associated with the original graph and in the fact that MS/BP equations are always exact and have a unique solution on trees[13].

**Definition 2.** Let  $\{\psi_{ij}\}$  be a MS fixed-point (10)-(11), and let  $\mathbf{d}, \mathbf{p}$  be the decisional

Name	MS(-5)		MS(-3)		LNDRC		DHEA	
	gap(%)	time(s)	gap(%)	time(s)	gap(%)	time(s)	$\mathrm{gap}(\%)$	time(s)
6p	2.2	3.5	2.6	0.6	4.2	0.5	2.2	21.3
6u	1.5	6.4	4.3	0.7	4.3	0.5	1.5	0.4
7p	2.3	90.2	3.9	1.7	7.7	1.5	2.3	6000.3
7u	2.2	134.1	2.2	1.8	3.6	1.2	2.2	596.4
8p	2.4	255.5	3.4	3.8	7.1	5.2	2.3	6004.2
8u	1.8	351.1	3.3	4.9	7.5	4.1	3.3	6000.9
9p	1.8	555.6	2.3	10.8	8.6	16.1	22.1	6000.0
9u	1.9	775.8	3.3	11.1	6.2	13.1	Not Found	6000.4
10p	1.7	1761.9	1.7	28.0	10.4	114.4	31.3	6000.5
10u	2.7	2468.4	2.7	32.2	7.7	59.8	Not Found	6000.6
11p	1.5	972.3	1.6	49.3	11.6	630.0	Not Found	6003.1
11u	2.2	5632.8	2.6	71.9	9.0	360.6	Not Found	6001.5
12p	1.5	4970.8	1.6	121.4	11.3	3507.7	Not Found	6009.8
12u	2.0	4766.7	2.4	174.1	10.0	1915.7	Not Found	6002.3
mean	2.0	1624.7	2.7	36.6	7.8	473.6	_	4760.1

Table III. Results H class

variables associated with this fixed point, i.e.  $(d_i^*, p_i^*) = \arg \max \psi_i(d_i, p_i)$  for the physical field  $\psi_i$  from (20). We will assume this maximum to be non degenerate. We will employ the *induced subgraph*  $S^*=(V^*, E^*)$  defined by  $V^* = \{i \in V : p_i^* \neq *\} \cup \{r\}$  and  $E^* = \{(i, p_i^*) : i \in V, p_i^* \in V\}$ . The cost of this subgraph is  $\mathcal{H}(S^*) = \mathcal{H}(\mathbf{p}) = \sum_{i \in V} c_{ip_i^*}$ .

The following optimality property of the MS-induced solution will be proven in the appendix.

**Theorem 3.** Given a MS fixed point  $\{\psi_{ij}\}$  on G (unbounded D) with induced subgraph  $S^* = (V^*, E^*)$  and any subtree  $S' = (V', E') \subseteq G$  with  $V' \subseteq V^*$ , then  $\mathcal{H}(S^*) \leq \mathcal{H}(S')$ 

This result has an easy generalization to loopy subraphs:

**Corollary 4.** With  $S^*$  as in Theorem 3, given any connected subgraph  $S' = (V', E') \subseteq G$  with  $V' \subseteq V^*$ , then  $\mathcal{H}(S^*) \leq \mathcal{H}(S')$ .

*Proof.* Apply Theorem (3) to a spanning tree of S'.

This trivially implies the following result of optimality of the MS solution in a particular case:

Corollary 5. With 
$$S^* = (V^*, E^*)$$
 as in Theorem 3, if  $V^* = V$  then  $\mathcal{H}(S^*) = PCST(G)$ 

In [5], the MGW algorithm includes two additional methods to obtain a better PCST solution: StrongPrune and Minimum Spanning Tree maintaining the same vertex set. Both methods give a substantial improvement boost to the MGW candidate computed in the first phase. A natural question may arise, does any of these two methods may help to improve the solution of MS? The answer is negative in both cases, and it is a trivial consequence of Theorem (3).

Corollary 6. 
$$MST(V^*, E \cap (V^* \times V^*)) = \mathcal{H}(S^*)$$

*Proof.* The minimum spanning tree of  $(V^*, E \cap (V^* \times V^*))$  satisfies the hypothesis of Theorem (3), so  $\mathcal{H}(S^*) \leq MST(V^*, E \cap (V^* \times V^*))$ . The converse inequality is trivially true due to the optimality of the MST.

Corollary 7. 
$$\mathcal{H}\left(StrongPrune\left(S^{*}\right)\right)=\mathcal{H}\left(S^{*}\right)$$

*Proof.* This is a consequence of the fact that  $V\left(\operatorname{StrongPrune}\left(S^{*}\right)\right)\subseteq V\left(S^{*}\right)=V^{*}$  and thus Theorem (3) applies, implying  $\mathcal{H}\left(S^{*}\right)\leq\mathcal{H}\left(\operatorname{StrongPrune}\left(S^{*}\right)\right)$ . The opposite inequality  $\mathcal{H}\left(\operatorname{StrongPrune}\left(F\right)\right)\leq\mathcal{H}\left(F\right)$  was proved in [5].

# VI. DISCUSSION

In this work we compared MSGSTEINER, an algorithm inspired in the Cavity Theory of Statistical Physics, with two state-of-the art algorithms for the Prize-Collecting Steiner Problem. The Cavity Theory is expected to give asymptotically exact results on many ensembles of random graphs, so we expected it to give better performance for large instances. The comparison was performed both on randomly-generated graphs and existing benchmarks. We observed that MSGSTEINER finds better costs in significantly smaller times for many of the instances analyzed, and that this difference in time and quality grew with the size of the instances and their solution. We find these results encouraging in views of

future applications to problems in biology in which optimization of networks with millions of nodes may be necessary, in particular given the conceptual simplicity of the scheme behind MSGSTEINER (a simple fixed-point iteration). Additionally, we showed some optimality properties of the Max-Sum (the equations behind MSGSTEINER) fixed points for the unbounded depth case: optimality in some limit cases, and optimality in the general case under the two forms of post-processing present in the MGW algorithm.

#### VII. ACKNOWLEDGEMENTS

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# Appendix A: Post-processing and optimality proofs

Before tackling the proof of the Theorem 3, we will need the following definitions and a technical result.

**Definition 8.** (Computation tree) The computation tree is a cover of the graph G, in the following sense: it is an (infinite) tree  $\mathcal{T}_G$  along with an application  $\pi: \mathcal{T}_G \to G$  that satisfies (a)  $\pi$  is surjective and (b)  $\pi_{|i\cup\partial i}: i\cup\partial i\to \pi$   $(i\cup\partial i)$  is a graph isomorphism for every  $i\in\mathcal{T}_G$ . It can be explicitly constructed as the graph of non-backtracking paths in G starting on a given node  $v_0$ , with two paths being connected iff the longest one is identical to the other except for an additional final node (and edge). Up to graph isomorphisms, this tree does not depend on the choice  $v_0$ .

The (finite) tree  $\mathcal{T}_G(t, v_0)$  is defined by the radius t ball centered around  $v_o$  in  $\mathcal{T}_G$ . Alternatively, it can be directly constructed as the graph of non-backtracking paths of length t starting on  $v_0$ , with two paths being connected iff the longest one is identical to the other except for an additional final node (and edge). Clearly the finite computation tree depends strongly on the choice of  $v_0$ 

For both computation trees, edge weights (and node prizes) will be lifted (transported) naturally as  $c_{ij} = c_{\pi(i)\pi(j)}$ .

Lifting edge constraints by  $g_{ij} = g_{\pi(i)\pi(j)}$  defines a (R, D)-PCSF problem with  $R = \pi^{-1}(\{r\})$  on  $\mathcal{T}_G$ . On  $\mathcal{T}_G(t, v_0)$  instead, it gives a slightly relaxed (R, D)-PCSF problem in

which leaf nodes can point to neighbors in G that are not present in  $\mathcal{T}_G$ . For convenience, let us extend  $\pi$  by setting  $\pi(*) = *$ .

Remark 9. As  $\mathcal{T}_G(t, v)$  is a tree, the MS equations are exact and have a unique fixed point in  $\mathcal{T}_G(t, v)$ [13].

**Lemma 10.** Any MS fixed point in a graph G can be naturally lifted to a MS fixed point in  $\mathcal{T}_G$ . Moreover, any MS fixed point can be naturally lifted to a MS fixed point over a slightly modified  $\mathcal{T}_G(t,v)$  with extra cost terms only on leaves.

Proof. As MS equations are local and the two graphs are locally isomorphic, given a fixed point  $\{\psi_{ij}\}_{(i,j)\in E}$ , the messages  $\Psi_{ij}=\psi_{\pi(i)\pi(j)}$  satisfy the fixed point equations on  $\mathcal{T}_G$ . On  $\mathcal{T}_G(t,v)$  the MS equations are satisfied everywhere except possibly on leaf nodes (where the graphs are not locally isomorphic). Given a leaf i attached with edge (i,j), add an energy term  $-E_i(d_ip_i)=\psi_{\pi(i)\pi(j)}(d_i,\pi(p_i))$ . Now MS equations are satisfied everywhere on for this modified cost function.

Now we proceed to prove Theorem 3

#### 1. Proof of Theorem 3

*Proof.* Assume S' oriented towards the root node r, i.e. defining a parenthood vector  $(p'_i)_{i \in V'}$ , such that  $E' = \{(i, p'_i) : i \in V' \setminus \{r\}\}$ . Consider the subgraph  $S = (V_S, E_S)$  of  $\mathcal{T}_G(N+1, r)$  induced by  $S^*$ , i.e. defined by  $V_S = \{v : \pi(v) \in V^*\}$ ,  $E_S = \{(i, j) : (\pi(i), \pi(j)) \in E^*\}$ .

It can be easily proven that the connected component in S of the root node of  $\mathcal{T}_G(N+1,r)$  is a tree S'' isomorfic to  $S^*$  (see [11]). Denote by  $\{p^*\}$  the decisional variables induced by  $S^*$  and by  $\{p'\}$  the ones induced by S'. The parenthood assignment

$$q_i = \begin{cases} p_i' & i \in V_{S''} \\ p_i^* & i \notin V_{S''} \end{cases}$$

satisfies  $q_i \neq *$  if  $q_j = i$  (as  $V' \subseteq V^*$ ) and so depths  $d_i$  can be assigned so as to verify all  $g_{ij}$  constraints in  $\mathcal{T}_G(N+1,r)$ . Now the cost associated with  $\mathbf{q}$  is  $\mathcal{H}(\mathbf{q}) = \sum_{i \in V_{S''}} c_{ip_i'} + \sum_{i \notin V_{S''}} c_{ip_i^*} \geq \sum_{i \in \mathcal{T}_G(N+1,r)} c_{ip_i^*} = \sum_{i \in V_{S''}} c_{ip_i^*} + \sum_{i \notin V_{S''}} c_{ip_i^*}$  due to the optimality of the MS solution  $\mathbf{p}^*$  in the computation tree (this is because MS is always exact on a tree). This implies clearly that  $\mathcal{H}(S^*) \leq \mathcal{H}(S')$ .

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