Sampling Subgraphs with Guaranteed Treewidth for Accurate and Efficient Graphical Inference

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ABSTRACT

How can we run graphical inference on large graphs efficiently and accurately? Many real-world networks are modeled as graphical models, and graphical inference is fundamental to understand the properties of those networks. In this work, we propose a novel approach for fast and accurate inference, which first samples a small subgraph and then runs inference over the subgraph instead of the given graph. This is done by the bounded treewidth (BTW) sampling, our novel algorithm that generates a subgraph with guaranteed bounded treewidth while retaining as many edges as possible. We first analyze the properties of BTW theoretically. Then, we evaluate our approach on node classification and compare it with the baseline which is to run loopy belief propagation (LBP) on the original graph. Our approach can be coupled with various inference algorithms: it shows higher accuracy up to 13.7% with the junction tree algorithm, and allows faster inference up to 23.8 times with LBP. We further compare BTW with previous graph sampling algorithms and show that it gives the best accuracy.

KEYWORDS

Markov networks, graph sampling, treewidth, graphical inference

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1 INTRODUCTION

Given a large graph whose nodes represent discrete random variables, how can we compute their posterior marginals efficiently? Graphical inference is a crucial task in data mining and machine learning, which has been applied to solve various node classification problems such as malware detection [8, 32], social network analysis [3, 13, 36], and recommender systems [5, 11].

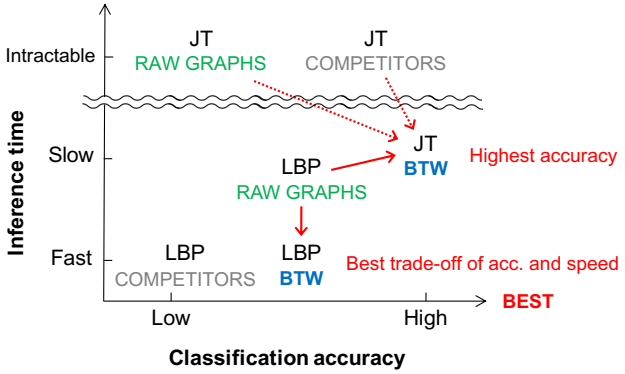

Figure 1: Advantages of BTW over other approaches. BTW a) gives the best accuracy when the junction tree (JT) algorithm is used, and b) speeds up the inference without hurting accuracy when LBP is used. JT is intractable except for the subgraphs from BTW.

Loopy belief propagation (LBP) [35] is an inference algorithm which has been used widely for the node classification. Yet, LBP has crucial limitations such that 1) it performs *approximate* inference rather than *exact* inference, and 2) its convergence is not guaranteed for general graphs; the conditions that LBP converges have been found only for restricted settings [12, 21]. These limitations have made it difficult to apply LBP to applications where the stability of inference is required. There are previous works [9, 10] that aim to solve the convergence problem by approximating LBP by a series of linear operations, but they lead to unstable accuracy since the amount of approximations is not bounded.

The junction tree algorithm [15] is an *exact* inference algorithm that does not suffer from the unstable convergence. However, this approach requires exponential time and space with the treewidth of a graph [15]; thus, efficient inference requires graphs with *bounded treewidth*. Although computing the treewidth of a graph is NP-complete [4], recent advances [23, 24, 28] in structure learning of Bayesian networks are able to learn from data a high-scoring graph that respects a given treewidth bound. This allows exact tractable inference on the learned graph. However, there are many applications where the graph is given, rather than learned: for instance, node classification in a citation network of research articles. In

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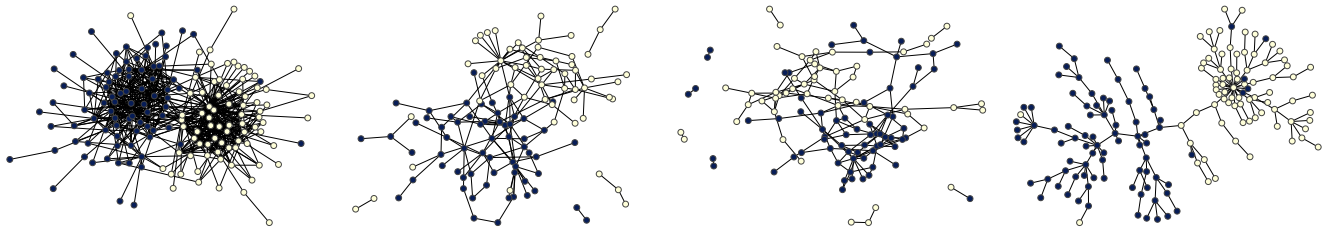


(a) Original graph. (TW ≈ 24) **(b) Sampled subgraph by RE.** (TW ≈ 8) **(c) Sampled subgraph by FF.** (TW ≈ 7) **(d) Sampled subgraph by BTW.** (TW = 1)

Figure 2: Guaranteed treewidth by BTW. (a) A web network of 163 blogs which are divided into two political groups. (b) The random edge sampling and (c) the forest fire sampling [17] generate subgraphs with 162 edges, which have disconnected components and large treewidth (≥ 7). (d) Our proposed bounded treewidth (BTW) sampling generates a connected subgraph with the same number of edges, but with bounded treewidth of 1 while preserving the separate political groups.

such cases, exact inference is intractable if there is no control of treewidth.

In this work, we propose a novel approach which allows efficient inference on large graphs. Our idea comprises two steps. First, we sample the original graph obtaining a bounded-treewidth subgraph. This is done by our proposed bounded treewidth (BTW) sampling, a novel algorithm to generate a subgraph with bounded treewidth while retaining as many edges as possible. Once we obtain the subgraph, we run on it a) exact inference by the junction tree algorithm or b) approximate inference by LBP based on a purpose. If we run the junction tree algorithm, our approach is more accurate than running LBP on the original graph, despite slow speed. We also have guaranteed convergence as the algorithm runs exact inference. If we run LBP, our approach shows similar accuracy with much faster computational time. These results are due to the success of our BTW sampling that maintains essential edges of the original graph with guaranteed bounded treewidth.

To the best of our knowledge, BTW is the first graph sampling algorithm that controls the treewidth of subgraphs and allows efficient graphical inference. The problem of generating subgraphs similar to an original graph has been studied widely in the data mining community [2, 17, 19], but none of the previous algorithms controls the treewidth of subgraphs. Furthermore, unlike other approaches that sample an edge at each iteration until the desired size is achieved, BTW selects cliques as minimal units, maintaining the essential neighborhood of each node. This gives every node a chance to preserve its comprehensive context and leads to improving the efficiency of graphical inference.

We evaluate our approach with the junction tree algorithm and LBP, which are the representative inference algorithms, on various real-world networks. As a result of extensive experiments, we demonstrate the following strengths of our approach:

- The junction tree algorithm on the subgraph generated from BTW achieves the highest accuracy, which is up to 13.7% higher than that from LBP on the original graph.
- LBP on the subgraph generated from BTW is up to 23.8× faster than LBP on the original graph, providing similar or even higher accuracy in some datasets.
- When we run LBP on subgraphs generated from BTW and other sampling algorithms, BTW shows up to 5.6% higher accuracy than the best competitors do.

These observations are summarized in Figure 1. BTW enables exact inference by the junction tree algorithm which is intractable in raw graphs and shows the highest accuracy. BTW also allows faster inference when LBP is used, while maintaining the original accuracy. The detailed experimental results are presented in Section 5.

Figure 2a shows BTW generates a subgraph with guaranteed treewidth on a web network of 163 blogs with two political groups. The previous random edge (RE) sampling and forest fire (FF) sampling generate subgraphs of Figures 2b and 2c, respectively, which contain disconnected components, noisy connections between the different groups, and large treewidth (≥ 7). On the other hand, BTW generates a connected subgraph of Figure 2d, which has low treewidth of 1 and preserves the separate political groups with the same number of edges as in Figures 2b and 2c. As a result, the junction tree algorithm is tractable only in the graph of Figure 2d, and LBP shows the best performance in that graph. The approximate treewidth is reported in (a) to (c) by the *min-fill-in* and *min-degree* heuristics, since the exact computation is intractable [6].

2 RELATED WORKS

We introduce related works for our proposed approach, which are categorized into treewidth, inference algorithms, and sampling algorithms. We denote an undirected graph by $G = (\mathcal{V}, \mathcal{E})$ where $\mathcal{V}$ and $\mathcal{E}$ represent the sets of nodes and edges, respectively.

2.1 Treewidth

Intuitively, the treewidth of a graph quantifies the extent to which it resembles a tree structure. We introduce the concepts of a clique and triangulation before defining formally the treewidth.

Definition 2.1 (Clique). Given a graph G, a set C of nodes is a *clique* if all of its nodes are pairwise connected. A clique of k nodes is called a k-clique and it contains $k(k-1)/2$ edges. A clique C is *maximal* if it is not a subset of a larger clique in the graph G.

Definition 2.2 (Triangulated graph). An undirected graph T is *triangulated* if all the chordless cycles existing in T are of length less than or equal to 3. Note that a chordless cycle is a cycle such

that no two nodes of the cycle are connected by an edge that does not belong to the cycle. *Triangulation* is the process of generating a triangulated graph from a graph G by inserting additional edges cutting all the cycles of length greater than 3 in G.

Definition 2.3 (Treewidth). The *treewidth* of a triangulated graph T is the number of nodes in its largest maximal clique minus one. The treewidth of a general graph G is the minimum treewidth among all possible triangulations of G.

Given a graph, it is intractable to compute its treewidth because it requires all possible triangulations [6]. Instead, the treewidth can be bounded to k if the graph is shown as a subgraph of a k-tree.

Definition 2.4 (k-tree). An undirected graph $K = (\mathcal{V}, \mathcal{E})$ is a *k-tree* of treewidth k if the addition of any edge $(u, v) \notin \mathcal{E}$ among its nodes $u, v \in \mathcal{V}$ increases its treewidth k, or it is a $(k+1)$-clique and thus no edge can be added. A subgraph of a k-tree is called a *partial* k-tree, and its treewidth is smaller than or equal to k.

We can generate a k-tree by the following inductive process [26]:

- **Base case:** a clique with $k+1$ nodes is a k-tree.
- **Inductive step:** given a k-tree K_n on n nodes, a new k-tree K_{n+1} is obtained by connecting a new node u to a k-clique C in K_n and generating k additional edges between u and C. This adds a new $(k+1)$-clique of nodes $\{u\} \cup C$ to K_n.

Learning a graphical model with bounded treewidth has been studied extensively. Karger and Srebro [14] have learned a Markov network that best represents given observations. Srebro [31] also has learned a Markov network that represents a probability distribution. For learning a Bayesian network instead of a Markov network, score-based learning with bounded treewidth has recently been addressed in [28, 29]. However, none of the previous approaches have used the idea of bounded treewidth learning to sample a subgraph that is suitable for efficient graphical inference.

2.2 Inference Algorithms

Belief propagation (BP) is an inference algorithm for Markov networks [35], which performs efficiently variable elimination. Given potentials of the variables in a graph, BP efficiently computes their posterior marginals by passing messages between the variables. BP computes the exact marginals when the graph is a tree. Otherwise, we run its variations described below.

Loopy belief propagation (LBP) is an approximate inference algorithm for cyclic graphs [35]. Unlike BP that passes the messages sequentially and only once following the tree structure, LBP updates all messages iteratively until convergence. However, since its convergence is not guaranteed, one needs to adjust the parameters to stabilize the termination of the algorithm, which are represented as a potential or an affinity matrix [8, 25]. There exist various approaches to guarantee its convergence by linear approximations, but the amount of approximation is not bounded [9, 10].

The *junction tree algorithm* is an exact inference algorithm for cyclic graphs [15]. It triangulates a given graph G and generates a supergraph T. Then, it finds the maximal cliques on T and builds a maximum weight spanning tree over the cliques where the weight between two cliques is the number of shared variables. We get the exact marginals by running BP on the resulting tree. However, its time and space complexities are exponential with the size of the largest maximal clique in T, which depends on how we triangulate G. Since finding an optimal triangulation is intractable, a typical approach is to revert to a heuristic approach whose quality is not guaranteed [7]. As a result, a tractable computation of the junction tree algorithm is not guaranteed on a general graph.

2.3 Graph Sampling

Graph sampling is a task of generating subgraphs that preserve the properties of a graph. Given an undirected graph $G = (\mathcal{V}, \mathcal{E})$, we aim to generate a subgraph $U = (\mathcal{V}', \mathcal{E}')$ such that $\mathcal{V} = \mathcal{V}'$ and $\mathcal{E}' \subset \mathcal{E}$. In this work, we focus on the *edge-sampling* which samples only the edges not changing the nodes. This is because our objective is to run graphical inference efficiently; each node is an essential variable which cannot be removed from the graph.

Graph sampling has been studied widely in data mining community. Leskovec and Faloutsos [17] compared different graph sampling algorithms and showed that the forest fire sampling [18] and the random walk sampling work well in maintaining the original properties. Li et al. [19] showed drawbacks of existing random walk based algorithms and proposed two novel methods. Some works focused on social networks. Wang et al. [34] compared various sampling algorithms on directed social networks. Voudigari et al. [33] proposed a sampling algorithm on social networks.

However, there has been no sampling algorithm that focuses on graphical inference. Most of the previous approaches sample subgraphs by selecting individual edges iteratively until the desired size is achieved, missing complex relationships between multiple nodes. On the other hand, our BTW sampling selects cliques as minimal units instead of edges to guarantee the bounded treewidth of subgraphs and to maintain the comprehensive neighborhood of each node. This leads to improved accuracy and efficiency of graphical inference on the generated subgraphs.

3 PROPOSED METHOD

We propose the bounded treewidth (BTW) sampling, a novel algorithm for generating subgraphs with bounded treewidth. BTW selects cliques as minimal units instead of edges to bound the treewidth, supporting tractable and accurate inference by the junction tree algorithm and preserving the context of each node.

Figure 2a shows a simple graph of 163 nodes with binary states, which is generated by slicing randomly a principal submatrix from the adjacency matrix of the PolBlogs network which we use in our experiments (Section 4). The two groups of nodes are separated clearly satisfying the property of homophily. BTW generates the subgraph in Figure 2d bounding its treewidth to 1, enabling accurate and efficient inference with only 39% of the edges.

3.1 Algorithm

The main objective of BTW is to guarantee the bounded treewidth of a sampled subgraph, which in turn leads to accurate and efficient inference on the graph. In other words, given a treewidth bound k, the treewidth of a subgraph U generated from BTW should be smaller than or equal to k. To achieve the objective, we keep track of a k-tree K along with U such that U is a subgraph of K. Thus, it is possible to bound its treewidth without exact computations.

Algorithm 1 Bounded treewidth (BTW) sampling

Require: a graph $G = (\mathcal{V}, \mathcal{E})$ and bound k
Ensure: a sampled subgraph U and a k-tree K
1: $K, U, H \leftarrow initialize(G, k)$ # H is a max-heap
2: **while** $|\mathcal{V}_U| < |\mathcal{V}|$ **do**
3: $u, C \leftarrow next\_node(H)$
4: $U \leftarrow (\mathcal{V}_U \cup \{u\}, \mathcal{E}_U \cup \{(u, v) | v \in \mathcal{N}_G(u) \cap C\})$
5: $K \leftarrow (\mathcal{V}_K \cup \{u\}, \mathcal{E}_K \cup \{(u, v) | v \in C\})$
6: $H \leftarrow update\_heap(H, u, C)$
7: **end while**
8: **return** U, K

BTW first selects $k+1$ nodes randomly to create an initial k-tree K, which is a $(k+1)$-clique, and creates the induced subgraph U from the same set of nodes. Then, BTW takes iterations of selecting a new node u by a score-based approach: given a score function $m(v, C)$ between a candidate node v and a clique C in K, it selects the node with the maximum score. BTW adds the selected node u to both K and U until all nodes are included in U.

Algorithm 1 describes the whole process of BTW. It initializes a k-tree K, a subgraph U, and max-heap H in line 1. The max-heap H is introduced to speed up the process and is discussed in Section 3.2. Then, BTW adds a new node u iteratively until all nodes are included in U, in lines 2 to 7. At each iteration, it selects u in line 3 and then updates U, K, and H in lines 4 to 6. BTW returns K along with U as a result in line 8, since K is a junction tree that is needed when running the junction tree algorithm over U.

3.1.1 Score Function. The simplest choice of the score function m is the uniform random function:

$$m(u, C) = \text{uniform}(0, 1). \tag{1}$$

Since it scores randomly all candidate nodes, using this function equals to first ordering all nodes randomly and then adding one node at a time following the order. However, it generates a sparse subgraph that maintains very few edges, because it does not take into account the structure of the original graph G.

Our main objective is to generate subgraphs that preserve the properties of G to support efficient graphical inference. Thus, we propose the following score function that is designed to maximize the number of edges in the sampled subgraphs:

$$m(u, C) = \sum_{v \in C \cap \mathcal{N}_G(u)} \left(w(u, v) + \text{uniform}(0, \alpha)\right), \tag{2}$$

where α is a small constant, and $w(u, v)$ is a positive weight of the edge between nodes u and v, assigned before running BTW.

This score function maximizes greedily the sum of edge weights in the subgraph U at every iteration. It simply maximizes the number of edges if w is a constant function, while one can design w to treat the edges differently. The uniform random function with the parameter α gives a randomness to the sampling process when the scores of multiple nodes are similar. For our experiments, we set w to a constant function as we deal with simple graphs, and α to a small value 10^{-4} to use it as a tie-breaker.

3.1.2 Subgraph Generation. BTW chooses randomly the first variable $u_1 \in \mathcal{V}$ and initializes the set $\mathcal{I}$ of sampled nodes:

$$\mathcal{I} = \{u_1\}. \tag{3}$$

Then, until $\mathcal{I}$ contains $k+1$ variables we add to it a new node u_i that maximizes the score, chosen from $\mathcal{V} \setminus \mathcal{I}$. Since we initially do not have a k-tree or a subgraph, we use $\mathcal{I}$ instead of a clique: the score function can be used generally with a node set.

$$u_i = \arg\max_{u \in \mathcal{V} \setminus \mathcal{I}} m(u, \mathcal{I}). \tag{4}$$

After that, BTW generates a complete graph K_{k+1} over the sampled $k+1$ nodes, which is a k-tree by construction. BTW generates also the induced subgraph U_{k+1} by selecting all the original edges whose incident nodes are both in $\mathcal{I}$. U_{k+1} is the initial subgraph which we update in the following iterations, and its treewidth is at most k since it is a subgraph of K_{k+1}.

Then, BTW takes iterations of adding a subsequent node u_{i+1} to the current subgraph U_i and k-tree K_i of i nodes, generating new graphs U_{i+1} and K_{i+1} of $i+1$ nodes. As in the initialization, BTW selects a node that maximizes the score function m as follows:

$$u_{i+1}, C_k^* = \arg\max_{u, C_k \subseteq K_i} m(u, C_k), \tag{5}$$

where C_k is a k-clique contained in K_i.

Given u_{i+1} and C_k^*, BTW first updates K_i by connecting u_{i+1} to C_k^*. This is the same as adding a new clique $C_k^* \cup \{u_{i+1}\}$ to K_i by considering a clique as a minimal sampling unit. However, it is not possible to add the same clique to U_i since some of the edges in the clique may not be included in the original graph G. Thus, we instead connect u_{i+1} only to $\mathcal{N}_G(u_{i+1}) \cap C_k^*$ to guarantee that U is a subgraph of G; note that K is not necessarily a subgraph of G as it is used only for bounding the treewidth of U. We repeat the iteration until all nodes are sampled, and return K and U.

3.1.3 Number of Sampled Edges. BTW aims to maximize greedily the number of edges in U while bounding its treewidth, using the score function of Equation (2). The function counts the number of edges that are added to U if u is connected to C. Thus, the number of edges in U_{i+1} is maximized as we find the maximum score for all pairs of nodes and cliques, and connect the selected pair by Equation (5) to create K_{i+1}. The number of sampled edges will be much less if the score function of Equation (1) is used.

It is possible to further limit the number of edges in U by any sampling algorithm as U already has bounded treewidth; the treewidth of any of its subgraphs is bounded to k. On the other hand, it is very difficult to increase the number of sampled edges, since it is likely that more edges lead to increased treewidth. Recall that it takes exponential time even to simply compute the treewidth of a graph. Thus, we leave it as a future work to increase the number of sampled edges from our subgraph U. It can be done from designing a new score function or by implementing a whole new algorithm coupled with more advanced techniques.

3.2 Optimization

It is redundant to compute the scores of all candidate nodes at each iteration since the scores of most nodes remain unchanged. Thus, we store in a max-heap the maximum score $s(u) = \max_{C \in K} m(u, C)$

of every candidate node u and optimize the algorithm by selecting the next node from the max-heap at each iteration.

We initialize $s(u)$ of every node u as zero. Then, at each iteration where a new clique C_{k+1} is added to the current k-tree K, we update the score $s(u)$ of every candidate node u as follows:

$$s(u) \leftarrow \max\left\{s(u), \max_{C_k \subset C_{k+1}} m(u, C_k)\right\}. \tag{6}$$

If $s(u)$ is updated, we store also the clique C_k with the maximum score since it is needed when adding u to the subgraph.

A naive approach is to update the scores of all nodes neighboring in C_{k+1}, since such nodes' scores with regard to C_{k+1} are greater than zero. The new scores need to be compared with their previous maximum scores. To expedite the update process, our optimization updates the scores of *only the neighbors of a new node* v which has been added to the current subgraph U. This results in the same update as in the naive approach, but is more efficient in orders of magnitude: it makes BTW run in linear time with the number of edges and scalable to large graphs.

Lemma 3.1 (Optimization). *When a new node v and a clique C_{k+1} of $k+1$ nodes are added to the current subgraph U and k-tree K, respectively, the score $m(u, C_k)$ of a node $u \notin \mathcal{N}_G(v)$ and a clique $C_k \subset C_{k+1}$ is less than or equal to the current score $s(u)$.*

Proof. We assume that α in Equation (2) is used only as a tie-breaker. The following holds because we assume $u \notin \mathcal{N}_G(v)$:

$$\max_{C_k \subset C_{k+1}} m(u, C_k) = m(u, C_{k+1} \setminus \{v\}).$$

Then, Equation (6) for computing the new maximum score $s(u)$ of node u is given as follows with regard to C_{k+1}:

$$s(u) \leftarrow \max\left\{s(u), m(u, C_{k+1} \setminus \{v\})\right\}. \tag{7}$$

Recall that C_{k+1} is formed by connecting v to a k-clique $C_k = C_{k+1} \setminus \{v\}$, existing already in K. Since all cliques in K have been used already to update the score of every candidate node which is not included in the current K, C_k has also been considered for updating $s(u)$ before we add v to K in this step. Thus, Equation (7) is a redundant operation that does not change $s(u)$. □

3.3 Theoretical Analysis

We further present theoretical analysis of BTW about its time complexity and preservation of connectivity. Lemma 3.2 shows that BTW has a linear scalability with the number of edges of the given graph. The effect of k^2 is negligible since we normally use a small treewidth bound k such as 2 or 4.

Lemma 3.2 (Time complexity). *Given a graph $G = (\mathcal{V}, \mathcal{E})$ and a treewidth bound k, the time complexity of BTW is $O(|\mathcal{E}|(k^2 + \log|\mathcal{V}|))$ with the optimization of Lemma 3.1.*

Proof. BTW selects a new node u at each iteration. The number of heap updates after selecting u is $O(|\mathcal{N}_G(u)|)$, and each update is $O(\log|\mathcal{V}|)$. The computation of Equation (6) to update each score is $O(k^2)$. Thus, the complexity of all heap updates is given as

$$O\Big(\sum_{u \in \mathcal{V}} |\mathcal{N}_G(u)|(k^2 + \log|\mathcal{V}|)\Big) = O(|\mathcal{E}|(k^2 + \log|\mathcal{V}|)).$$

Table 1: A summary of four real-world networks that we use in our experiments. All datasets are publicly available.

Network	Nodes	Edges	Labels
Wikipedia[1]	35,579	495,357	16
CoRA[2]	23,567	91,965	10
PubMed[3]	19,717	44,324	3
PolBlogs[4]	1,222	16,714	2

The computational cost for heap deletions is safely ignored with a natural assumption of $|\mathcal{V}| \leq |\mathcal{E}|$, since it is $O(|\mathcal{V}|\log|\mathcal{V}|)$. □

BTW preserves the connectivity of the original graph in sampled subgraphs. This is especially useful for graphical inference because disconnected nodes in a graphical model are considered independent from each other, which is not true for most real-world networks. In such cases, evidence is not propagated to all nodes, decreasing the accuracy of classification.

Lemma 3.3 (Connectivity preservation). *When a given graph G is connected, all intermediate subgraphs during the iterations of BTW are connected, including the one to be returned.*

Proof. We prove the lemma by mathematical induction:

(1) **Base case.** The initial nodes in $\mathcal{I}$ are guaranteed to be connected because every node is selected for maximizing the number of edges of the subgraph U when added to $\mathcal{I}$.
(2) **Inductive step.** We assume that the subgraph U_i of i nodes is connected. Then, the next subgraph U_{i+1} with an additional node u becomes disconnected only if there exists no edge between the nodes in U_i and the rest of G, since u has been selected for its maximum score among the candidates. However, that cannot happen since G is connected. Thus, U_{i+1} is connected.

Thus, every subgraph generated by BTW is connected. □

4 EXPERIMENTAL SETTINGS

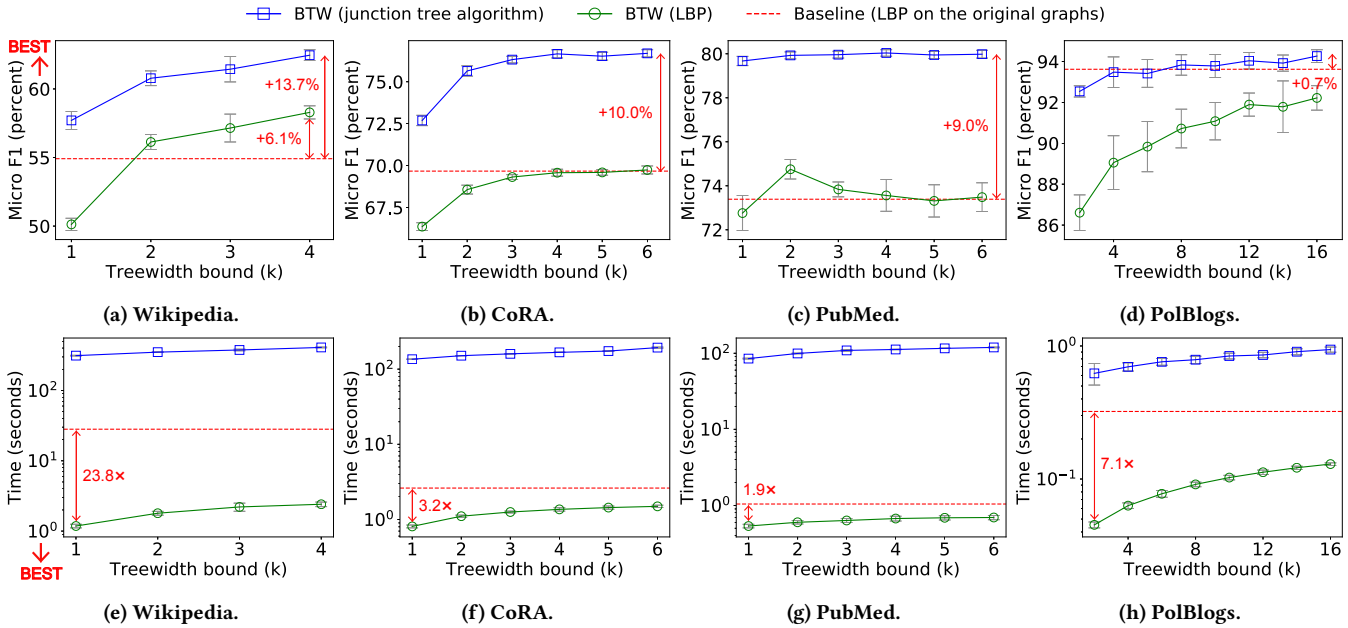
In this section, we present experimental settings: datasets, competitors, etc. Our experiments were done by a workstation with Intel Xeon E5-2630 2.20GHz CPU and 50GB memory.

4.1 Datasets

We use four real-world networks summarized in Table 1. Wikipedia is a crawled dump of Wikipedia pages from 16 top level categories of the computer science domain [22]. The nodes represent pages, and the edges represent hyperlinks. CoRA and PubMed are citation networks whose nodes represent research articles, and edges represent citations [22, 30]. Each node is labeled according to the research topic in which it falls into. PolBlogs is a web network whose nodes represent political blogs (liberal or conservative ones), and edges represent hyperlinks [1].

Some of the networks were originally directed. Thus, we model them as undirected by removing the edge directions as done in [20].

[1] https://github.com/sharadnandanwar/snbc
[2] https://github.com/sharadnandanwar/snbc
[3] https://linqs-data.soe.ucsc.edu/public/Pubmed-Diabetes.tgz
[4] http://www-personal.umich.edu/~mejn/netdata/polblogs.zip



(a) Wikipedia. (b) CoRA. (c) PubMed. (d) PolBlogs.

(e) Wikipedia. (f) CoRA. (g) PubMed. (h) PolBlogs.

Figure 3: Micro F1 scores of node classification and inference time by the junction tree algorithm (the solid blue lines) and LBP (the solid green lines) over the subgraphs sampled by BTW, and the baseline (LBP over the original graph, shown by red dashed lines). BTW with the junction tree algorithm achieves the highest accuracy, despite its slow inference time. On the other hand, BTW with LBP shows comparable accuracy to the baseline with much faster inference.

We also remove the isolated components since they are independent in terms of inference. The numbers of nodes and edges in Table 1 are counted after these preprocessing steps.

4.2 Graph Sampling Algorithms

We compare BTW with other graph sampling algorithms. We focus on edge sampling approaches that sample only edges, since every node is an essential target variable which we aim to classify.

Random edge (RE) sampling is the simplest algorithm that samples repeatedly an edge uniformly at random. However, it selects most edges from high-degree nodes, ignoring the importance of low-degree nodes. Random node-edge (RNE) sampling solves the problem by selecting a node uniformly at random and sampling one of its adjacent edges. Hybrid (HYB) approach [16] combines the two approaches: it performs either a step of RE or RNE randomly with a probability p at each iteration. p is set to 0.8 as in [16].

Random walk (RW) sampling uniformly at random picks a node and then simulates a random walk with restart. It selects all edges that its random walker passes through. Random jump (RJ) sampling is similar to RW, but the random walker restarts randomly in any node instead of the starting one. Frontier sampling (FS) [27] uses multiple random walkers simultaneously to generate more stable subgraphs. Forest fire (FF) sampling [18] selects n neighbors instead of one at each step, where n follows a probability distribution.

Because none of the methods guarantees to keep the original connectivity in subgraphs, we propose two additional algorithms BTW-W and BTW-J by modifying RW and RJ, respectively. They guarantee the connectivity of a sampled subgraph by generating a spanning tree of nodes using BTW of $k = 1$ and then selecting the remaining edges by their original algorithms (RW and RJ). We use those approaches to demonstrate that the superior performance of BTW comes from not only its ability to keep the connectivity, but also its idea of sampling cliques instead of edges.

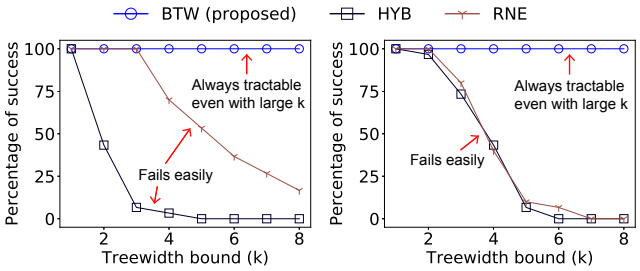
Table 2: The average numbers of edges of subgraphs generated from BTW, with respect to the treewidth bound k.

Network	$k = 1$	$k = 2$	$k = 4$	$k = 8$	$k = 16$
Wikipedia	35,578	57,896	84,213	126,234	165,620
Cora	23,566	36,307	46,158	51,310	54,479
PubMed	19,716	23,109	25,169	26,641	27,619
PolBlogs	1,221	2,004	3,086	4,477	6,374

4.3 Node Classification by Inference

The real-world networks in Table 1 are not graphical models and thus contain no probabilistic information. For solving node classification by graphical inference, we model each dataset as a pairwise Markov random field (MRF), an undirected graphical model that has been widely used for node classification [8]. Compared with a standard MRF that requires a potential for every clique existing in a graph, a pairwise MRF uses only pairwise potentials, which we call *edge potentials*, and thus the modeling process is simple.

It is important to choose proper potentials since they determine the properties of a graphical model. Given the number n of states, we generate an edge potential matrix ψ of size $n \times n$ for each dataset based on the observed evidence as follows. First, we initialize ψ as



(a) PubMed. **(b) PolBlogs.**

Figure 4: Ratios of successful runs (no out of memory error) of the junction tree algorithm for subgraphs from BTW and major competitors (HYB and RNE). BTW maintains the success ratio of 100%, while the others easily fall into memory shortages as k increases.

a zero matrix. Then, for each connected pair of observed nodes in the graph, we add one to the corresponding element of the matrix based on their labels. After that, we normalize ψ by the sum of its elements to make it represent a probability distribution. The resulting potentials are shown to follow the homophily (details in Appendix A). However, we have found that LBP does not converge with the computed potentials since they are too skewed. For this reason we introduce a new parameter d that alleviates the skewness of the potentials and use it in all experiments where LBP is used (details in Appendix B). We use the original potentials when applying the junction tree algorithm since it is a deterministic algorithm and has no such problem.

For each network and sampling algorithm we generate 10 subgraphs with different random seeds. Then, we adopt the 3-fold cross validation for each subgraph: we hide the labels of 1/3 of the nodes and predict them by running graphical inference using the rest as evidence. Then, we find the maximum-a-posteriori (MAP) assignments as predicted labels from posterior distributions computed from the inference. We evaluate the result using micro and macro F1 scores as done in [22] but report only the micro F1 scores due to the lack of space. We report the averages in all experiments.

5 EXPERIMENTAL RESULTS

In this section, we present experimental results which answer the following questions about BTW:

- Q1. **Accuracy and inference time (Section 5.1).** What are the accuracy and inference time on the subgraphs from BTW compared with those on the original graphs?
- Q2. **Comparison with other sampling algorithms (Section 5.2).** Is BTW more suitable for the graphical inference compared with the other sampling algorithms?
- Q3. **Optimization of BTW (Section 5.3).** How much speedup can be obtained by the optimization of BTW? How does it scale with the number of edges and the treewidth k?

5.1 Accuracy and Inference Time

Figure 3 shows how the classification accuracy and inference time change if we run the inference algorithms on the subgraphs from BTW instead of the original graphs. The junction tree algorithm

Table 3: Micro F1 scores of LBP on the subgraphs from BTW and the competitors when the treewidth bound k is 2. BTW shows the best accuracy in all datasets.

Method	Wikipedia	CoRA	PubMed	PolBlogs
RE	35.3 ± 0.2	57.9 ± 0.3	61.8 ± 0.4	75.8 ± 1.0
RNE	51.3 ± 0.3	65.2 ± 0.2	71.1 ± 0.1	84.4 ± 0.6
HYB	49.4 ± 0.2	64.5 ± 0.2	69.8 ± 0.3	83.4 ± 0.4
RW	26.5 ± 2.7	43.0 ± 1.7	56.5 ± 1.2	65.2 ± 3.4
RJ	36.6 ± 0.4	55.4 ± 0.3	63.2 ± 0.4	75.6 ± 0.5
FS	29.8 ± 0.2	47.9 ± 0.2	56.2 ± 0.5	72.4 ± 0.8
FF	49.4 ± 0.2	63.7 ± 0.3	62.8 ± 0.4	79.8 ± 0.9
BTW-W	50.9 ± 1.4	66.8 ± 2.4	69.7 ± 0.7	82.4 ± 1.7
BTW-J	53.0 ± 0.3	67.5 ± 0.2	73.6 ± 0.8	85.0 ± 1.3
BTW	**56.1 ± 0.5**	**68.6 ± 0.3**	**74.8 ± 0.4**	**86.6 ± 0.9**

achieves up to 13.7% higher accuracy than the baseline (LBP on the original graph), showing consistent improvements in most cases; the exception is PolBlogs with small k, but the accuracy improves with k even in this case and outperforms the baseline from $k = 8$. Although the inference is slower than the baseline due to the overhead of computing the joint probability of each clique by the junction tree algorithm, it is still tractable because BTW guarantees to generate subgraphs with bounded treewidth.

The accuracy of LBP on the subgraphs is generally similar to the baseline. This implies that BTW successfully captures essential relationships between nodes, and thus LBP is able to recover the original accuracy with less edges: the subgraphs of Wikipedia when $k = 2$ contain only 11.7% of the original edges as shown in Table 2. At the same time, LBP on the subgraphs is consistently faster than the baseline from 1.5× to 23.8× based on the value of k.

We use small treewidth bounds in CoRA and Wikipedia (up to 6 and 4, respectively) in order to keep the junction tree algorithm tractable, which requires large memory of $O(n^k)$, where n represents the number of states [15]. Recall that n in both graphs are much larger than in the other graphs. However even in this case BTW yields an important improvement over the baseline.

5.2 Comparison with Other Approaches

We compare BTW and the other graph sampling algorithms by the classification accuracy on generated subgraphs. Most competitors require to know in advance the number of edges that the subgraph should contain, while BTW finds the subgraph automatically once k is specified. Thus, we first run BTW with a given bound k, record the number of edges that are present in the subgraph, and let the others generate subgraphs with the same numbers of edges.

Recall that the time and space complexities of the junction tree algorithm are both exponential with k. Usually it is not possible to run exact inference on subgraphs generated without any control of the treewidth. This causes the junction tree algorithm to fail with an out-of-memory error. The percentages of successful inference (no out-of-memory) on PubMed and PolBlogs are shown in Figure 4. They decrease sharply for all methods other than BTW, especially when $k > 3$, while the inference is always successful on the subgraphs returned by BTW due to the bounded treewidth.

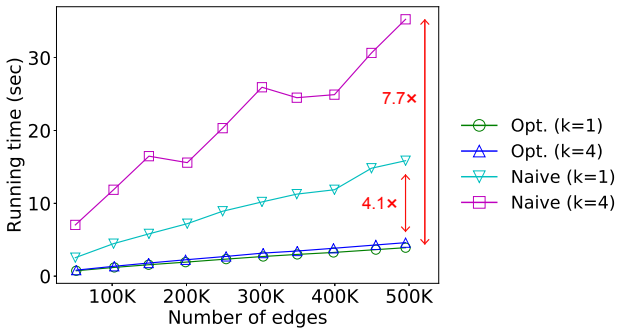


Figure 5: Sampling time of BTW on graphs of different numbers of edges and treewidth bound k. *Opt.* and *Naive* represent BTW with and without the optimization, respectively. BTW runs up to 7.7 × faster with the optimization, showing near linear scalability as presented in Lemma 3.2.

(a) CoRA **(b) Wikipedia**

Figure 6: The potential matrices of CoRA and Wikipedia. The nodes in those graphs have the homophily as the diagonal elements are significantly larger than the others.

We then perform node classification on such subgraphs reverting to LBP and obtain the accuracy in Table 3. BTW consistently shows the best accuracy compared with all competitors. It is notable that BTW performs better than BTW-J and BTW-W that keep the original connectivity in subgraphs by running BTW of $k = 1$ before other sampling algorithms. This implies that the superior performance of BTW does not rely on its property of keeping the connectivity, but on its main ideas of bounding the treewidth and providing each node a chance of having a neighborhood of size k: every node keeps essential relationships in sampled subgraphs.

5.3 Optimization of BTW

Figure 5 shows the running time of BTW on graphs with different numbers of edges, with and without the optimization in Lemma 3.1. We have sampled nine principle submatrices from the adjacency matrix of Wikipedia for creating graphs of different sizes. BTW shows near linear scalability with the number of edges as discussed in Lemma 3.2. It also shows the effect of optimization: introducing it makes BTW up to 7.7 times faster than before. Thus, BTW can be used efficiently for running inference in large graphs.

6 CONCLUSION

In this work, we propose the bounded treewidth (BTW) sampling, a novel graph sampling algorithm that generates subgraphs with guaranteed bounded treewidth. BTW samples as many edges as possible while bounding the treewidth, selecting cliques as minimal units of sampling and thus preserving the comprehensive neighborhood of each node. The subgraphs generated from BTW make the junction tree algorithm tractable by the bounded treewidth, which shows up to 13.7% higher micro F1 in node classification than loopy belief propagation (LBP) does on the original graph. Moreover, BTW speeds up LBP up to 23.8 times with accuracy comparable to that on the original graph, and consistently higher than those from the other sampling algorithms. We expect that subgraphs generated from BTW are suited to other applications which can exploit the low treewidth. Future works include extending BTW to heterogeneous networks by introducing new score functions that consider various types of nodes, edges, and additional attributes.

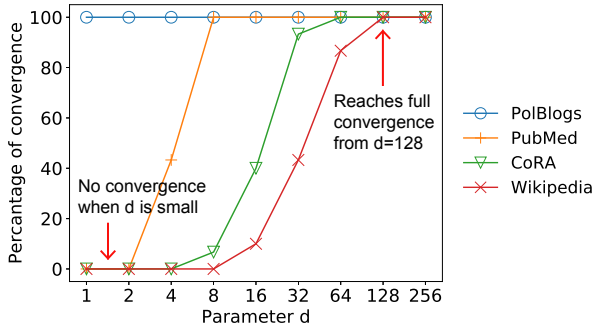


Figure 7: Percentages of runs that LBP converges by different values of d. LBP hardly converges with small d on three of the four datasets, and the convergence ratios increase as d increases: all ratios become 100% if $d \geq 128$.

A POTENTIAL MATRICES

The following matrices ψ_B and ψ_M show the potentials of PolBlogs and PubMed, respectively, that are generated from the process of modeling MRFs in Section 4.3:

$$\psi_B = \begin{bmatrix} 0.437 & 0.047 \\ 0.047 & 0.469 \end{bmatrix}, \quad \psi_M = \begin{bmatrix} 0.118 & 0.042 & 0.019 \\ 0.042 & 0.356 & 0.038 \\ 0.019 & 0.038 & 0.329 \end{bmatrix}.$$

Figure 6 shows the potentials of CoRA and Wikipedia by representing the values as colors (the bigger, the darker). The diagonal elements in all those matrices are significantly larger than the others, implying that the nodes are positively correlated and follow the assumption of homophily.

B CONVERGENCE OF LBP

An exact condition that LBP converges has not been presented in the literature. Thus, we empirically show that LBP converges more often when the potential matrix is less skewed. We introduce a new parameter d which controls the skewness of a potential: a potential matrix ψ is replaced by a weighted average $\frac{1}{d}(\psi + (d-1)M)$ with a constant matrix M, whose elements are uniform and sum to one. Thus, the potentials become less skewed as d increases.

For each dataset, we run LBP ten times with different sets of observed nodes and show in Figure 7 the percentage of runs that converge. We conclude it as a convergence when the maximum difference between the messages in two consecutive iterations is within 10^{-4} before 1000 iterations. As a result, it is shown that LBP

hardly converges in three of the four datasets when d is a small value such as 2 or 4. The convergence seems especially difficult on CoRA and Wikipedia, which contain larger numbers of labels compared with the other datasets. The convergence ratios become 100% for all dataset when d is at least 128.

Based on this result, we set d to 256 when LBP is used, to guarantee a full convergence. On the contrary, it is not necessary to use d when the junction tree algorithm is used because the convergence is guaranteed: it stops after one iteration of fully propagating the observed information. This is an important advantage of running exact inference on subgraphs from BTW because it is not necessary to modify the relationships arbitrarily, which leads to different marginals from the ones that can be inferred from a network.

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