Fast Search of Subgraphs Discriminative for Classification and Regression

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Abstract

Recently, in various fields such as computational chemistry and bioinformatics, attention has been paid to classification and regression in which the inputs are graphs of arbitrary size and shape. Whether a certain subgraph is included or not is the most fundamental feature for graphs that have no direct descriptors available. However, enumerating subgraph patterns and learning any models using them are so expensive since the number of possible subgraph patterns are intractably large due to the combinatorial explosion. Currently, discriminative pattern mining has been studied and given a good solution to this problem. The previous search method for such discriminative subgraph patterns tries to find the best one by the depth first search with some pruning rules. Such a exact search, however, is costly for heavily repeated use, which is necessary to obtain the number of features enough for high performance classifiers or regressors. To overcome this computational cost issue, we propose two approximate algorithms based on (i) best first search, (ii) Monte Carlo Tree Search(MCTS). We demonstrate effectiveness of our proposed methods by comparing performance in real problems using QSAR datasets.

1 Introduction

Graphs are fundamental data structures for representing combinatorial objects such as chemical compounds, networks and others. However, precisely because of their combinatorial nature, it is usually difficult to understand the underlying trends in large datasets of graphs. In addition, due to the rapid increase in the amount of data in recent years, supervised learning in which the inputs are graphs of arbitrary size and shape has attracted attention in the fields of computer vision [1–4], chemoinformatics [5–13], bioinformatics [14–16] and computational chemistry [17, 18]. and natural language processing [19].

For this problem, the most fundamental feature is subgraph indicators because many reactions and events are attributed to substructures. How-

ever, the number of all possible subgraph patterns is intractably large due to the combinatorial explosion, it is difficult to make feature from dataset. Therefore, it is necessary to make feature by restricting the subgraph based on some criterion. Frequent subgraph mining [20,21] is one of these methods and is often used. However, since this method only considers the frequency, it is possible to overlook the important features for learning. On the other hand, discriminative pattern mining [8, 22, 23] extracting features important for learning using model-based discriminative criteria has been studied. Based on these methods, the present paper considers efficient discriminative subgraph pattern search methods.

1.1 Related Work

Related works [8,23] search the discriminative subgraph pattern using depth first policy and branch and bound method. While these methods perform efficient searches by designing tricky pruning, search policy of depth first is naive and they still suffer from computational costs for some domain or large datasets.

1.2 Our Approach

To overcome the above difficulty, we consider the more efficient search algorithms using Best First Search and Monte Carlo tree search(MCTS). These methods are known to be effective in some domains, and in this paper we apply to subgraph search domain.

2 Preliminaries

2.1 Notations

Let $[n]$ be $\{1, 2, \ldots, n\}$, and let $\mathbb{I}(P)$ denote the indicator of P, i.e., $\mathbb{I}(P) = 1$ if P is true, else 0. A labeled graph is represented in a 4-tuple $G = (V, E, \mathcal{L}, l)$, where V is a set of vertices, $E \subset V \times V$ is a set of undirected

edges, $\mathcal{L}$ is a set of labels, and $l : V \cup E \to \mathcal{L}$ is a mapping that assigns each vertex and edge to a label. We denote as $G \sqsupseteq g$ the subgraph isomorphism and its negation as $G \not\sqsupseteq g$. Thus, a subgraph indicator $\mathbb{I}(G \sqsupseteq g) = 1$ if $G \sqsupseteq g$, otherwise 0. We also denote the training set of input graphs $G_i \in \mathcal{G}$ and output responses $y_i \in \mathcal{Y}$ as

$$\mathcal{D} = \{(G_1, y_1), (G_2, y_2), \ldots, (G_N, y_N)\}, \tag{1}$$

where $\mathcal{G}$ is a set of all finite-size, connected, discretely-labeled, undirected graphs. We denote $\mathcal{G}_N = \{G_i \mid i \in [N]\}$, and the set of all possible connected subgraphs as $\mathcal{S}_N = \bigcup_{G \in \mathcal{G}_N} \{g \mid G \sqsupseteq g\}$.

Definition 1 *(subgraph isomorphism) Let* $G' = (V', E', \mathcal{L}', l')$ *and* $G = (V, E, \mathcal{L}, l)$*,* G' *is subgraph isomorpic to* G *iff there exist an injective mapping* $\phi : V' \to V$*, s.t., (1)* $\forall v \in V, l(v) = l'(\phi(v))$*, (2)* $\forall (v_1, v_2) \in E, (\phi(v_1), \phi(v_2)) \in E'$ *and (3)* $l(v_1, v_2) = l'(\phi(v_1), \phi(v_2))$*.*

2.2 Search Space for Subgraphs

In supervised learning from graphs, we represent each input graph $G_i \in \mathcal{G}_N$ by the characteristic vector $(\mathbb{I}(G_i \sqsupseteq g) \mid g \in \mathcal{S})$ with a set $\mathcal{S}$ of relevant subgraph features. However, since $\mathcal{S}$ is not explicitly available when the learning phase starts, we need to simultaneously search and construct $\mathcal{S}$ during the learning process. In order to define an efficient search space for $\mathcal{S}_N$, i.e., any subgraphs occurring in $\mathcal{G}_n$, the techniques for *frequent subgraph mining* are useful. Note that any subgraph feature $g \in \mathcal{S}_N$ can occur multiple times at multiple locations in a single graph, but $\mathbb{I}(G_i \sqsupseteq g) = 1$.

In the present paper, we use the search space of the gSpan algorithm [20], which performs a depth-first search on the tree-shaped search spaces on $\mathcal{S}_N$, referred to collectively as an *DFS code tree*, as shown in Figure 1. Each node of the DFS code tree holds a subgraph feature g' that extends the subgraph feature g at the parent node by one edge, namely, $g' \sqsupseteq g$.

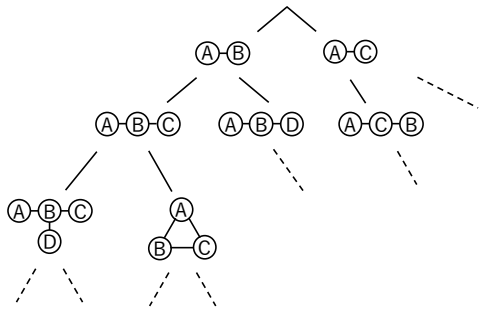


Figure 1: DFS code tree

The following *anti-monotone* property of subgraph isomorphism over the DFS code tree on $\mathcal{S}_N$ can be used to derive the efficient search-space pruning of the gSpan algorithm:

$$G_i \not\supseteq g \Rightarrow G_i \not\supseteq g' \quad \text{for} \quad g' \sqsupseteq g. \tag{2}$$

2.3 Discriminative Criteria

Assume we have a two-class problem ($y_i \in \{-1, +1\}$). We evaluate the discriminating degree of each subgraph by the following formulas. When predicting the graph labels with discrete values, $ClassificatonScore$ ($CScore$) is used defined as (3).

$$CScore(g) = \max\Big[\sum_{n=1}^{N} y_n(2\mathbb{I}(G_n \sqsupseteq g) - 1), \sum_{n=1}^{N} y_n(2\mathbb{I}(G_n \not\supseteq g) - 1)\Big] \tag{3}$$

This score is the sum of the values that take +1 if the graph label prediction is correct and -1 otherwise. When predicting the graph labels with real values, $RegressionScore$ ($RScore$) is used defined as (4).

$$\begin{aligned} RScore(g) &= \mathrm{MSE}(\mathcal{D}_1(g)) + \mathrm{MSE}(\mathcal{D}_0(g)) \\ \mathrm{MSE}(\mathcal{D}) &= \frac{1}{N}\sum_{i\in[N]}(y_i - \bar{y})^2,\ \bar{y} = \frac{1}{N}\sum_{i\in[N]} y_i. \end{aligned} \tag{4}$$

where MSE is mean squared error, and $\mathcal{D}_1(g) = \{(G_i, y_i) \in \mathcal{D} \mid G \sqsupseteq g\}$ and $\mathcal{D}_0(g) = \{(G_i, y_i) \in \mathcal{D} \mid G \not\supseteq g\}$.

3 Problem Setting and Challenges

In this paper, the problem is to search for a subgraph that maximizes (3) or minimizes (4). However, the search space of subgraphs (Section 2.2) is intractably large due to the combinatorial explosion. The naive search policy require very high computational costs and it is difficult to find the suitable solution. Our challenge is to design a efficient search policy for subgraphs in a large search space based on the discriminative criteria.

4 Depth First Search with Branch and Bound

State of the art methods [8, 23] searching for a discriminative subgraph pattern is based on the depth first search, as shown in Figure 2 (a), with branch and bound. [8] searches the best subgraph patttern using $CScore$. This method calculates the bound of child node of search space, and if the bound is lower than the provisional solution the child is pruned.

Theorem 1 *Given $\mathcal{D}_1(g)$ and $\mathcal{D}_0(g)$, for any subgraph $g' \supseteq g$,*

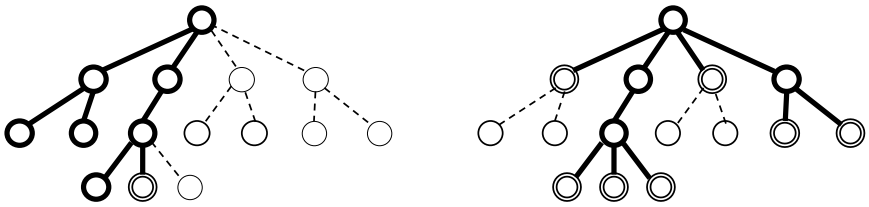
$$CScore(g') \leq \max\left[2\sum_{\{n|y_n=+1,D_1(g)\}} y_n - \sum_{n=1}^{l} y_n, -2\sum_{\{n|y_n=-1,D_1(g)\}} y_n + \sum_{n=1}^{l} y_n\right] \tag{5}$$

the bound is calculated based on $RegressionScore$ and used for pruning.

Theorem 2 *Given $\mathcal{D}_1(g)$ and $\mathcal{D}_0(g)$, for any subgraph $g' \supseteq g$,*

$$RScore(g') \;\geq\; \min_{(\diamond,k)} \Big[\mathrm{MSE}(\mathcal{D}_1(g) \setminus S_{\diamond,k}) + \mathrm{MSE}(\mathcal{D}_0(g) \cup S_{\diamond,k})\Big] \tag{6}$$

where $(\diamond, k) \in \{\leq, >\} \times \{2, \ldots, |\mathcal{D}_1(g) - 1|\}$, and $S_{\diamond,k} \subset \mathcal{D}_1(g)$, such that $S_{\leq,k}$ is a set of k pair (G_i, r_i) selected from $\mathcal{D}_1(g)$ in descending order of residual error r_i, and $S_{>,k}$ is that in increasing order. Note that $\setminus$, $\cup$ are set difference and set union respectively.



(a) Depth First Search (b) Best First Search

Figure 2: Where the bold circles show already searched nodes and double circles show the candidate nodes for next expansion

5 Proposed Method

The previous method employs a simple search policy with depth first without using the discriminative criterion value $(CScore, RScore)$ of each node. In some cases, this criteria is useful for designing search policies. In this section, using this criteria, we present two efficient methods to search a discriminative subgraph pattern based on (i) Best First Search and (ii) Monte Carlo Tree Search.

5.1 Best First Search

Best First search [24] is a search policy that expand from the best node based on some evaluation value, shown as Figure 2 (b). The A* and Dijkstra algorithms, well known as route search algorithms, are also one of best first search and is known as very good search methods in some domains.

The previous method designed the pruning rule by calculating the bound value (5)(6). In the proposed method, this bound value is set as the search priority of each node, and is applied to the best first search. The procedure of the proposed algorithm is illustrated with pseudocode in Alg. 1. The search is started from the root node, and the node with the highest bound is selected from the expansion candidate set. The child nodes of the selected node are expanded, and the score is calculated and added to the expansion

candidate set. The above operation is repeated until pruning is possible for all expansion candidate set.

Alg. 1: Subgraph Search by Best First Search

Input: Training data $\mathcal{D} = \{(G_1, r_1), (G_2, r_2), \ldots, (G_N, r_N)\}$

Output: Best score subgraph g^*

Function *Best First Search($\mathcal{D}$)*

```
candidate ← {root} repeat
    g ← arg max_{candidate c} bound(c) ;
    candidate ← candidate/g ;
    forall child c of g do
        if Score(c) is better than score* then
            score* ← Score(c) ;
            g* ← c ;
        end
        candidate ← candidate ∪ c ;
    end
until all candidate can be pruned;
return g* ;
```

5.2 Monte Carlo Tree Search

We consider applying Monte Carlo tree search(MCTS) [25–27] to this problem. MCTS is widely known as a search planning method used in computer Go, and is used not only as a game playing algorithm but also in various fields such as feature selection. One of them, Upper Confidence Bounds for Tree(UCT) algorithm [25] is empirically known as a way to get better solutions within a limited costs. This method resolves the exploration-exploitation problem using Upper Confidence Bound(UCB), which allow to estimate the expected reword of each child. The simplest UCB policy is called UCB1 and does not require the prior specific knowledge. The policy

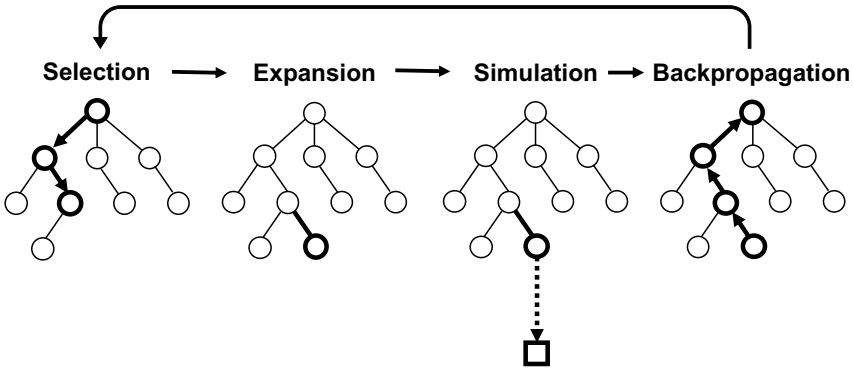


Figure 3: Four iterative operations of UCT

selects to search child node i that maximizes

$$UCB1 = \bar{X}_i + C \times \sqrt{\frac{2 \ln n}{n_i}} \tag{7}$$

where $\bar{X}_i$ is the average reward from child node i, n_i is the number of times child node i was selected, n is the number of times parent node of i was selected, and C is an exploration constant. The left term encourages the exploitation of high expected reward child, and the right term encourages the exploration of less visited child.

The UCT algorithm is an iterative method doing the four operations of selection, expansion, simulation, and backpropagation up to a predefined computational cost, shown as Figure 3.

1) Selection:

   Start from the root node, and select the child repeatedly until the expandable node is reached based on the value of (7). A node is expandable if it represents a non-terminal state and has unvisited children.

2) Expansion:

   One random child node that is unvisited is expanded. In this operation, we consider the same pruning condition as (5) or (6). If the

random select node can be pruned, another node is reselected and added.

3) Simulation:

A Monte Carlo simulation is run from the new expanded node, and repeatedly select a child from the available children uniformly and randomly. This simulation stops if the simulation node has no children or is based on a stochastic condition known as a stopping feature used in [26]. The stochastic condition is $1 - q^d$ depending on the simulation node level d, where $q < 1$ is a parameter and $q = 1 - 10^{-1}$ in the present paper.

4) Backpropagation:

Calculate the reword of the node g obtained by simulation. To align the range to $[0, 1]$, reward is defined,

$$reword(g) = \begin{cases} CScore/|\mathcal{D}| \\ -RScore/\mathrm{MSE}(\mathcal{D}) \end{cases} \tag{8}$$

these value will be large if discrimination is successful, otherwise small. Then backpropagate this reward to the nodes selected in selection and expansion phase.

Low Cost Simulation

In this problem setting, the search space is not given in advance. Therefore, we need to construct a search space that matches the given dataset and subgraph search at the same time. When Monte Carlo simulation is performed in this problem, it is necessary to enumerate all the child nodes for each simulation node, which requires a large cost. We design a low-cost simulation method since the simulation cost has a big influence on the search efficiency.

First, a graph including simulation node is randomly selected from the dataset. Expand the subgraph represented by the simulation node on the

selected graph. If an expanded subgraph is available(minimum order defined by [20]), this simulation is taken, otherwise it is repeated.

The entire procedure of the proposed algorithm is illustrated with pseudocode in Alg. 2, 3.

Alg. 2: Subgraph Search by UCT

Input: Training data $\mathcal{D} = \{(G_1, r_1), (G_2, r_2), \ldots, (G_N, r_N)\}$

Output: Best score subgraph g^*

Function *UCT($\mathcal{D}$)*

```
repeat
    g ← Selection(root) ;
    g ← Expansion(g) ;
    if Score(g) is better than score* then
        score* ← Score(g) ;
        g* ← g;
    end
    s ← Simulation(g) ;
    Backpropagation(s, g) ;
until predefined cost is exhausted;
return g* ;
```

Alg. 3: Four Operations in UCT

Function *Selection(g)*

while g *is expandable* **do**

$g \leftarrow \underset{children\ c\ of\ g}{\arg\max}\ \bar{X}_c + C \times \sqrt{\frac{2 \ln n_g}{n_c}}$;

end

return g ;

Function *Expansion(g)*

repeat

$g' \leftarrow random(\{children\ c\ of\ g\})$;

until *g' is not pruned*;

return g' ;

Function *Simulation(g)*

$s \leftarrow g$;

while s *has some child and not enough stochastic condition* **do**

repeat

$G \leftarrow random(\mathcal{D})$;

$s' \leftarrow random\ expansion\ from\ s\ on\ G$;

until s' *is enough to minimum order*;

$s \leftarrow s'$;

end

return s ;

Function *Backpropagation(s, g)*

$X = Score(s)$;

while $g \neq NULL$ **do**

$n_g \leftarrow n_g + 1$;

$\bar{X}_g \leftarrow \frac{\bar{X}_g \times (n_g - 1) + X}{n_g}$;

$g \leftarrow parent\ of\ g$;

end

6 Experiments

6.1 Datasets

We also evaluate the performance based on the most typical benchmark on real datasets: the quantitative structure-activity relationship (QSAR). We select Four binary-classification datasets (CPDB, Mutag, AIDS(CAvsCM), CAS) in Table 1: CPDB and Mutag for mutagenicity tests and AIDS(CAvsCM) for antiviral tests. All chemical structures are encoded as molecular graphs using RDKit[1], and some structures in the raw data are removed by chemical sanitization[2]. We simply apply a node labeling by the RDKit default atom invariants (edges not labeled), i.e., atom type, # of non-H neighbors, # of Hs, charge, isotope, and inRing properties. These default atom invariants use connectivity information similar to that used for the well-known ECFP family of fingerprints [28]. See [17] for more elaborate encodings.

Table 1: Dataset summary

Dataset	CPDB	Mutag	AIDS(CAvsCM)	CAS
# data	684	188	1503	4337
# $(y = +1, -1)$	(341, 343)	(125, 63)	(422, 1081)	(2401, 1936)
# nodes	25.2	26.3	59.0	30.3
# edges	25.6	28.1	61.6	31.3

# of nodes and edges are average.

[1] `http://www.rdkit.org/`

[2] Due to this pre-processing, the number of datasets differs from that in the simple molecular graphs in the literature, where the nodes are labeled by atom type, and the edges are labeled by bond type.

6.2 UNDER CONSTRUCTION

7 Conclusion

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