VERSACH: Finding Statistically Significant Subgraph Matches using Chebyshev’s Inequality

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ABSTRACT
Approximate subgraph matching, which is an important primitive for many applications like question answering, community detection, and motif discovery, often involves large labeled graphs such as knowledge graphs, social networks, and protein sequences. Effective methods for extracting matching subgraphs, in terms of label and structural similarities to a query, should depict accuracy, computational efficiency, and robustness to noise. In this paper, we propose VERSACH for finding the top-k most similar subgraphs based on 2-hop label and structural overlap similarity with the query. The similarity is characterized using Chebyshev’s inequality to compute the chi-square statistical significance for measuring the degree of matching of the subgraphs. Experiments on real-life graph datasets showcase significant improvements in terms of accuracy compared to state-of-the-art methods, as well as robustness to noise.

CCS CONCEPTS
• Information systems → Information systems applications; Data mining;

KEYWORDS
Subgraph Similarity, Approximate Matching, Statistical Significance, Chi-Square, Labeled Graph, Chebyshev’s Inequality

1 INTRODUCTION
With the growth of Open Linked Data in the form of knowledge graphs, social networks, bioinformatic structures, and road networks, efficient graph mining poses a challenging problem [2, 45]. Such large data sources are represented as labeled graphs, where entities are modeled as vertices, while their relationships are captured by edges, with labels defining the attributes of entities and relations.

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Figure 1: Two-hop neighborhood similarity based computation of χ² statistical significance for vertex match in VERSACH.

Subgraph querying is used across several domains including frequent pattern search in data mining [30], community detection in IR [24], question answering in NLP [36], object recognition in computer vision [6], and route planning [10]. The problem of subgraph match querying entails the extraction of subgraphs from an underlying graph having similar structure and labels to a given query [29, 33].

Traditional approaches for exact structural and label matching based on isomorphism are computationally infeasible. Thus, approaches based on pruning [26, 39, 50], indexing [42, 44], filtering [8, 20], and dynamic programming [22] have been proposed. However, they fail to scale for modern web-scale graph applications, wherein approximate subgraph matching was explored [29, 31] to extract similar subgraphs, with exact matches or with slight variations in structural elements and label mismatches. For example, in bioinformatics, approximate subgraph matching enables the detection of candidate regions in genome, that might have undergone abnormal mutations, for studying the associated medical effects [43, 51]. Although approximate subgraph extraction have been well studied [3, 18, 29, 31, 44, 47], efficiently finding matching subgraphs with improved runtime and accuracy remains an important problem. The problem of approximate subgraph matching aims to find the top-k subgraphs of Q that are best matching (maximum similarity) to Q in terms of vertex label and edge overlap. In our context, VERSACH finds the top-k statistically significant subgraphs of G as the best approximate matches of Q.
State-of-the-art. (Sub-)graph matching has been extensively studied, and the existing body of work can be broadly categorized into two groups – exact methods and approximate heuristics. Since graph isomorphism is quasi-polynomial [4] and subgraph isomorphism is NP-complete [12], earlier works on exact graph matching such as Swift-Index [42], VF2 [13, 26], PathBlast [28], SAGA [47], IsoRank [44] and GraphGrep [20] to name a few, explored pruning and indexing techniques. To tackle incomplete and noisy data, approximate matching techniques tolerate small amounts of structural and label mismatches. These methods usually rely on identifying candidate vertices, whose neighborhoods are then progressively expanded in a greedy manner – providing compute efficiency, although with possibly sub-optimal results. Initial approaches like TALE [48], variance [238], we have

\[ |X - \mu| \geq t \cdot \delta \leq 1/t^2 \]

for any \( t > 0 (t \in \mathbb{R}) \). Intuitively, the degree of label and structural overlap (i.e., similarity) between a query and its matching subgraph would demonstrate significant deviations (due to high similarity) from the expected distribution. Chebyshev’s inequality can be used to characterize the difference in terms of the number of standard deviations away from the mean to compute the statistical significance of candidate matching subgraphs. Such techniques have been studied for sequence mining [15, 16, 41], substring matching [14], subgraph similarity [1, 18], and clique finding [17].

Contributions. In this paper, we propose the Vertex Neighborhood Aggregation for Statistically Significant Subgraphs via Chebyshev Inequality (VERSACHI) algorithm for efficient top-k subgraph matching based on statistical significance. We identify candidate neighborhood regions matching an input query by using two-hop label and structural overlap based similarity. The deviation of the observed similarity, from the underlying distribution is then characterized by Chebyshev’s inequality and represented as symbols. Based on statistical significance, matching candidate regions are identified and explored in a greedy manner, to obtain the best matching subgraph to the query. Observe that VERSACHI adopts the methodology of [17] for finding subgraph matches, while differing from [18] in symbolic computation and neighborhood similarity. Initial empirical results on real and synthetic datasets showcase our proposed framework to outperform existing techniques in accuracy and robustness to noise.

2 VERSACHI ALGORITHM

This section describes the VERSACHI algorithm for extracting the top-k best approximate matching subgraphs from a target graph \( G = (V_G, E_G, L_G) \), with respect to a query graph \( Q = (V_Q, E_Q, L_Q) \). The working of VERSACHI comprises the following steps. The first 5 steps are offline and are done only once for a target graph, while the last 4 are online and take place when a query arrives.

1. Index Creation. Given a target graph \( G \), VERSACHI initially constructs two indexing lists summarizing the labels of the vertices and their neighbors. The first is an inverted list, \( I_G \), that maps vertex labels to the corresponding list of vertices having the label. The second index, the label neighbor list, \( LNL_G \), stores the link information of the neighbors for each vertex in \( G \). A label count vector index, \( LCV_G(u) \), for each vertex \( u \in G \) is also constructed. It stores the count of occurrence of each label (for \( |I'| \) labels) in the neighborhood of \( u \). This enables efficient computation of similarity between vertices as described next (step 4 onwards).

2. Similarity Measure. For a vertex pair \((u, v)\) we use a modified Tversky index \( t(u, v) \) to define the vertex similarity score \( \eta(u, v) \):

\[
\eta(u, v) = \frac{|N(u) \cap N(v)|}{(|N(u) \cap N(v)| + |N(v) \cap N(u)|^\delta)}
\]

where \( N(u) \) is the set of labels in the neighborhood of \( u \) including the label of \( u \) itself. Observe, by setting \( \delta = 1 \), we obtain the original Tversky index with \( \alpha = 0 \) and \( \beta = 1 \). Intuitively, the similarity of \( u \in G \) is maximized w.r.t. \( v \in Q \) when all neighbor labels of \( v \) are present in the neighbors of \( u \) (i.e., \( N(v) \subseteq N(u) \)). Since the presence of additional neighbors of \( v \in G \) should not affect the similarity, we set \( \alpha = 0 \) in the Tversky index. In essence, Eq. (1) captures the neighborhood recall of \( v \in Q \) provided by \( u \in G \) (thus, \( \beta = 1 \)). The exponential penalty factor, \( \gamma \), penalizes increasing mismatches in the neighborhood label overlap between vertex pairs. It captures fine differences in the neighborhoods by accentuating even smaller mismatches. Empirically, \( \gamma = 3 \) gave the best results.

3. Initialization. Using \( LCV_G(u) \) structures and similarity measure, VERSACHI computes the vertex similarity scores for every vertex pair in \( G \). This captures the underlying distribution. The expected similarity distribution across random neighborhoods of \( G \) is captured via 3 characteristics computed using \( \eta(u, w) : \forall u \in G, w \in G \).

(a) \( \psi(G) = \sum_{u, w \in G} \eta(u, w)/|V_G| \) : average vertex similarity score for all vertex pairs in \( G \)

(b) \( \delta(G) = (\sum_{u, w \in G} (\eta(u, w) - \psi(G))^2 / (|V_G| - 1))^{1/2} \) : standard

\[ \text{S}(X, Y) = \frac{|X \cap Y|}{|X|^{\alpha}|Y|^{\beta}} \]

for sets \( X \) and \( Y \) with parameters \( \alpha, \beta \geq 0 \).
deviation of the vertex similarity scores of $G$, and
(c) $\Delta(G) = \max_{u,w \in G} \{ |\eta_{u,w} - \psi(G)|/\delta(G) \}$: maximum deviation of vertex similarity score from the average among all the vertex pairs in terms of standard deviations in $G$.

4. Symbol Categorization. The degree of matching between a target graph vertex and a query vertex is captured in VersSachi by the amount of deviation of the vertex pair similarity score (in terms of the number of standard deviations) from the underlying expected distribution (computed above). The standard deviations are discretized using the step size parameter, $\kappa$. It also determines the total number of possible symbols, $\tau = \lceil (\Delta(G) - 1)/\kappa \rceil$. The set of category symbols, therefore, is $\Sigma = \{\sigma_1, \sigma_2, \ldots, \sigma_\tau\}$. Smaller values of $\kappa$ is preferred for differentiating between finer-grained structural mismatches.

For a pair of vertices $u$, $w$, its similarity is characterized using the symbol $\sigma_1$, $1 \leq i \leq \tau$. The first symbol, $\sigma_1$, spans the range of standard deviations up to $1 + \kappa$, i.e., $\sigma_1 : 0 \leq |\eta_{u,w} - \psi(G)|/\delta(G) < 1 + \kappa$. Subsequent symbols cover step size standard deviations each, $\sigma_i : 1 + (i - 1) \cdot \kappa \leq |\eta_{u,w} - \psi(G)|/\delta(G) < 1 + i \cdot \kappa$ for $2 \leq i \leq \tau$.

5. Expected Probabilities of Symbols. The expected probability of occurrence associated with the category symbols is next computed using the Chebyshev’s inequality. Observe, the deviation of vertex pair similarity from the mean can be in negative or positive direction. Since we are interested in vertices that have higher similarity than the mean (to capture higher matching), we only discretize the similarity (into symbols) when it is greater than the mean. For all similarities that are lesser than the mean, we fold them into symbol $\sigma_1$. Thus, assuming symmetric one-sided Chebyshev’s inequality, the occurrence probability of symbol $\sigma_i$ is $Pr(\sigma_i) = \frac{1}{2} \lceil \frac{1}{1+(i-1) \cdot \kappa} \rceil - \frac{1}{2} \lceil \frac{1}{1+i \cdot \kappa} \rceil$ for $2 \leq i \leq \tau$, and $Pr(\sigma_1) = 1 - \sum_{j=2}^{\tau} Pr(\sigma_j)$.

We also empirically evaluated the variant where the deviation in both the positive and negative side of the mean is considered (i.e., without folding). However, it produced no changes in our results. Since a very low similarity (large negative deviation) can potentially have large chi-square values and, thus, produce false matching results, VersSachi uses the onesided version.

Note that all the above steps are offline operations and performed only once for a target graph $G$.

6. Candidate Pair Mapping. Upon arrival of a query graph $Q$, the online processing starts with the construction of indexes $IL_Q$, $LNL_Q$, and $LCV_Q$, analogously to $G$. For each label in $Q$, VersSachi creates candidate pairs between the vertices of $G$ and $Q$ having the same label. These candidate pairs form the initial seed vertex for extracting matching subgraphs (to the query) via greedy neighborhood search. Formally, the candidate pairs generated are $CP = \{(v \in G, q \in Q) | L_G(v) = L_Q(q)\}$.

7. Vertex Symbol Sequence. For a candidate pair $(v \in G, q \in Q)$, VersSachi computes the vertex pair similarity score, $\eta(v, q)$, and characterizes the similarity score by assigning a category symbol based on the deviation from the expected similarity distribution (as discussed previously). The category symbol $\sigma_{(v,q)}$ captures the one-hop neighborhood similarity for vertices $v$ and $q$ (see Eq. (1)).

We next compute “second-order” candidate pairs between the vertex sets adjacent to $v$ and $q$. A greedy best matching based on the vertex pair similarity score is used to compute the second-order candidate pairs. Similar to $(v, q)$, each second-order candidate pair is assigned a category symbol based on the deviation of its similarity score from the expected. The initial category symbol $\sigma_{(v,q)}$ is aggregated with the second-order category symbols to form the vertex symbol sequence, $O_{(v,q)}$, for the candidate pair $(v, q)$.

As an example, consider Fig. 1 depicting an initial candidate pair between vertices $v_1$ and $q_1$ (both having label $A$) with category symbol $\sigma_1$ assigned to it (using Eq. (1)). The adjacent vertices of $v_1$ ($v_2, v_3, v_4$) and the neighbors of $q_1$ ($q_2, q_3, q_4$) are greedily best-matched based on vertex pair similarity to obtain the “second-order” candidate pairs. For instance, $v_2$ and $q_2$ provide the best match with the same label and the same neighborhood labels and, thus, forms the next candidate pair (with, say, category symbol $\sigma_2$). Subsequently, $v_3$ and $q_3$ are matched having the same label and partial neighborhood overlap (consider to be assigned symbol $\sigma_3$). Finally, the candidate pair $(v_4, q_4)$ is obtained with category symbol $\sigma_4$. The corresponding vertex symbol sequence, $O_{(v_4,q_4)} = \{\sigma_1, \sigma_2, \sigma_3, \sigma_4\}$, is assigned to $(v_4, q_4)$, captures the two-hop similarity between the candidate pair vertices $v_1$ and $q_1$ (Fig. 1).

8. Statistical Significance. The computed symbol sequence $O_{(v,q)}$ signifies the degree of matching between the two-hop neighborhoods of $v$ and $q$. Assuming $d$ to be the degree of $q$, since mapping is performed for the neighbors of $q$, the length of $O_{(v,q)}$ is $d$. Thus, the expected occurrence counts of category symbol $\sigma_i$ is $E[\sigma_i] = d \cdot Pr(\sigma_i)$. The observed occurrence counts of the category symbols are directly obtained from $O_{(v,q)}$. Using the observed and expected counts, VersSachi computes the chi-square statistics $\chi^2_{(v,q)}$ for all the candidate pairs obtained in CP (see step 6).

9. Approximate Matching. The candidate pairs along with their computed chi-square values, $(v, q, \chi^2_{(v,q)})$, are inserted into a primary max-heap structure. The candidate pair with the largest $\chi^2$ value is extracted (assume $(v, q)$) for initializing the top-1 matching subgraph, $Match^{(1)}$, and is considered as the starting seed vertex for greedy expansion to find matching subgraph region for the query $Q$.

Next, candidate pairs between the adjacent vertices of the extracted seed pair $(v, q)$ are constructed (as in step 6) and pushed into a secondary max-heap structure. As before, the vertex symbol sequence of the candidate pairs in the secondary heap are constructed, their statistical significances computed, and the pair with the highest $\chi^2$ value is extracted and added to $Match^{(1)}$. This process is iterated till the secondary heap is empty, or the size of $Match^{(1)}$ equals the number of vertices in $Q$. The subgraph obtained in $Match^{(1)}$ is reported as the top-1 best approximate matching subgraph for $Q$.

Vertices extracted from the primary and secondary heaps are marked as “done” to prevent duplicate entries in the heap structures, and ensuring that the same region is not repeatedly explored. To retrieve more top-$k$ approximate matches for a query, the secondary heap is reset and the process is re-run, starting from picking the currently best candidate pair (with highest statistical significance) from the primary heap. This is repeated until $k$ matches are obtained.

Complexity Analysis

Assume graph $G$ to contain $n$ vertices, $m$ edges and $|\Gamma|$ unique labels. Index construction (offline phase) requires $O(n)$ space for $IL_G$, $O(m)$ for $LNL_G$, $O(n \cdot |\Gamma|)$ for $LCV_G$, and $O(\tau)$ for symbol probabilities. The overall space complexity of VersSachi, therefore, is $O(n + m + n \cdot |\Gamma|)$. The time taken for index construction are $O(n)$ for $IL_G$, and $O(m)$ for both $LNL_G$ and $LCV_G$. Computing the target
Table 1: (a) Summary of the datasets characteristics. (b) Overall accuracy and runtime performance of the algorithms on the different datasets.

| Dataset | # Vertices | # Edges | # Unique Labels |
|---------|------------|---------|-----------------|
| Human   | 4,674      | 86,282  | 44              |
| HPRD    | 9,460      | 37,001  | 307             |
| Protein | 43,471     | 81,044  | 3               |
| Flickr  | 80,513     | 5,976   | 195             |
| IMDb    | 428,440    | 1,713   | 22              |

| Dataset | Algorithm | Human | HPRD | Protein | Flickr | IMDb |
|---------|-----------|-------|------|---------|--------|------|
|         | VELSET    | 0.42  | 0.65 | 0.37    | 0.75   | 0.53 |
|         | G-Finder  | 0.45  | 0.12 | 0.47    | out of memory | 0.55 |
|         | VersaCHI  | 0.90  | 0.81 | 0.67    | 0.84   | 0.87 |

| Value of Step Size (κ) | exact nEAdd nEDel nLabel nV Add nVDel |
|------------------------|----------------------------------------|
| 0.001                  | exact nEAdd nEDel nLabel nV Add nVDel |
| 0.01                   | exact nEAdd nEDel nLabel nV Add nVDel |
| 0.1                   | exact nEAdd nEDel nLabel nV Add nVDel |
| 1.0                   | exact nEAdd nEDel nLabel nV Add nVDel |

3 EXPERIMENTS

In this section, we discuss the empirical setup and evaluation of the VersaCHI algorithm, and its comparison to existing approaches. **Datasets.** We evaluate the performance of the algorithms on real datasets from 3 different domains: (i) Biological Networks: protein-protein interaction graphs of Human, HPRD [5] and Protein [40]; (ii) Social Interaction: social interaction network between users of the image and video hosting site Flickr, with the label of each user (vertex) denoting the group that she belongs to [40]; and (iii) Knowledge Graph: IMbd [40] containing named-entities like movies, actors, etc., along with their relationships. The characteristics of the datasets are shown in Table 1(a). Synthetically generated Barabási-Albert graphs are also used to study the scalability of VersaCHI.

**Query.** Query graphs (connected) are constructed (from the dataset) by initially selecting a random vertex, and exploring its neighborhood till |Q| vertices are visited. These are referred to as exact queries. To study the performance of the algorithms in presence of noise, exact query graphs were perturbed by introducing structural and label noise randomly by (i) modifying vertex labels (nLabel), or (ii) inserting or deleting vertices (nVAdd and nVDel resp.), or (iii) adding or deleting edges (nEAdd and nEDel resp.). The number of perturbations are limited to 2. Further, for each scenario, we generate queries with sizes varying from 3 to 13 (at intervals of 2), with 20 query graphs extracted for each size. Thus, for each dataset, we consider (6 × 6 × 20) = 720 queries, and report average results.

**Evaluation.** The efficiency of the algorithms is measured in terms of edge retrieval accuracy (using the labels of end vertices), that is, the fraction of edges of the query graph Q that are present in the matching subgraph retrieved. Additionally, we report the average runtime required (per query) by the different approaches to extract the approximate matching subgraphs. Since the introduced perturbations do not exist in the original graph, the exact query (for
obtaining the noisy query) is considered as the ground truth. For Barabási-Albert graphs we use exact queries only.

**Baselines.** We compare the performance of VERSACHI against the following: (i) VELSET [18], a statistical significance based approach for exploring candidate regions with partial label match; and (ii) G-Finder [33], a graph traversal based indexing for dynamic filtering and refinement of candidate match neighborhoods.

**Index.** The maximum index size taken by VERSACHI in our experiments is 1.4 GB for the Flickr graph, while the highest offline computation time is 37283.44 seconds, for IMDB dataset.

**Setup.** All experiments were implemented in C++ and were conducted on an Intel(R) Xeon(R) 2.60GHz CPU ES-2697V3 with 500GB of RAM. G-Finder was obtained from github.com/thiuliuliullh/GFinder and evaluated on a Visual Studio 2015 C++ platform.

**Empirical Results**

From Table 1(b), we observe that VERSACHI has a significantly better accuracy than the competing algorithms for finding the best matching subgraphs with more than 20% accuracy improvements (averaged across varying query types and sizes). The run-time of VERSACHI is slightly more than the other approaches due to the two-hop neighborhood similarity computation. In absolute terms, though, it is quite practical. Overall, with a slight increase in compute time, VERSACHI offers a substantial accuracy gain. (G-Finder crashes due to out-of-memory issues for Flickr and IMDB datasets.)

Fig. 2 depicts the performance for different query types. (Results on the other datasets are similar and are, thus, omitted due to space constraints). VERSACHI achieves better accuracy across all the different query types, with slight increase in runtime. Fig. 3 shows that with increase in query size, the runtime increases linearly (across query types), while the accuracy remains largely unaffected.

Fig. 4 studies the scalability of VERSACHI using synthetic Barabási-Albert graphs. The runtime is seen to increase linearly, with increase in number of vertices and average degree, conforming to the analysis of Sec. 2. The accuracy of VERSACHI is unaffected in these scenarios. With increase in the step size $\kappa$, accuracy decreases, as the number of symbols decreases, limiting the power of VERSACHI to differentiate between finer differences in neighborhood mismatches between the graphs, while the runtime remains mostly constant.

**4 CONCLUSIONS**

This paper proposed a scalable and highly accurate algorithm, VERSACHI, for approximate labeled graph querying. It shows significantly better accuracy than the competing methods across datasets and noise. Our framework is generic enough to accommodate other similarity measures and application-dependent tail distributions.

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