Experimental Evaluation of Counting Subgraph Isomorphisms in Classes of Bounded Expansion

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Abstract
Counting subgraph isomorphisms (also called motifs or graphlets) has been used extensively as a tool for analyzing biological and social networks. Under standard complexity assumptions there is no polynomial time algorithm for this problem, which limits the applicability of these tools to large data sets. Recent techniques from parameterized complexity have led to an algorithmic framework for isomorphism counting whose worst case time complexity is linear in the number of vertices, provided that the input graph has certain structural characteristics, known as bounded expansion. Previous work has suggested that the restrictions of bounded expansion structure—locally dense pockets in a globally sparse graph—naturally coincide with common properties of real-world networks such as clustering and heavy-tailed degree distributions. However, there has been little work done in implementing and evaluating the performance of this algorithmic pipeline. To this end we introduced CONCUSS, an open-source software package for counting subgraph isomorphisms in classes of bounded expansion. Through a broad set of experiments we evaluate implementations of multiple stages of the pipeline and demonstrate that our structure-based algorithm can be up to an order of magnitude faster than a popular algorithm for isomorphism counting.

1 Introduction
The analysis of complex networks has proven useful for understanding relationships between entities in large data sets. For example, networks modeling social interactions, protein functionality, and accessible transportation routes have been studied extensively in the network science community. However, since many network properties that might yield interesting insights are NP-hard to compute, the prevailing strategies for detecting such properties generally depend on sampling, estimation, and/or heuristics whose reasons for success or failure are not theoretically well understood.

At the same time, the structural graph theory and parameterized algorithms communities have a large body of literature on exactly solving NP-hard problems in polynomial time on sparse graphs by exploiting the underlying graph structure. Unfortunately, many of these results either rely on structure like low treewidth, which is unlikely to occur in many complex networks, or hide enormous constants in big-O notation that in practice negate the theoretical gains from the polynomial run times. Recent work has identified a structural classification of graphs known as bounded expansion that gives significant algorithmic advantages [6, 8], while accommodating the structural characteristics of complex networks [7]. Though there are some algorithms for bounded expansion that appear to be suitable for practical use, they have yet to be implemented and tested in order to understand their behavior.

In this work, we focus on algorithms for subgraph isomorphism counting, in which the number of occurrences of a small subgraph $H$ (sometimes called a motif or graphlet) in a larger host graph $G$ is counted. Because previous research has suggested that subgraph isomorphism counting can be used a building block for understanding network dynamics [22] and aligning similar graphs [10], an improved counting algorithm would have many practical applications. Our main contribution is a set of computational experiments using CONCUSS [17], an open source software tool written in pure Python that implements the best known algorithm for subgraph isomorphism counting in bounded expansion graphs [7]. On a high level, CONCUSS finds a coloring of the vertices to identify the relevant structure, uses the coloring to decompose the graph into small pieces, counts the isomorphisms on each small piece, and combines the sub-solutions to get a final count. Notably, the description of this pipeline leaves room for multiple choices for implementing certain subroutines; CONCUSS implements several variants for some of these routines.

Our experimental design is oriented towards two primary goals: (1) evaluating the extent to which CONCUSS is currently competitive with existing algorithms
for subgraph isomorphism counting and (2) identifying bottlenecks in the algorithmic pipeline of CONCUSS to guide further theoretical research. Theoretical advances to this pipeline would not only enable faster subgraph isomorphism counting, but also provide an improved framework for solving other combinatorial problems in graphs of bounded expansion (see Section 3.5). To these ends, our experiments answer four questions:

Q1. What choices of subroutines give the best performance in CONCUSS?
Q2. How does CONCUSS compare to other algorithms for subgraph isomorphism counting?
Q3. How does the distribution of color class sizes influence downstream performance?
Q4. Would alternative coloring types incur significant penalties in the downstream subroutines?

After giving the necessary background and notation in Section 2, we briefly describe the algorithmic pipeline CONCUSS implements in Section 3. Section 4 details the general experimental setup. In Section 5 we show the performance of various configurations of CONCUSS compared to each other (Q1) and to the NetworkX [10] implementation of the popular VF2 algorithm [5] (Q2). We then investigate in Section 6 ways in which theoretical improvements to the coloring algorithms might improve CONCUSS (Q3 and Q4).

2 Background

All graphs in this paper are assumed to be simple and undirected unless otherwise specified. For a graph $G$, let $V(G)$ and $E(G)$ denote the vertices and edges of $G$, respectively, and let $uv$ denote an edge with endpoints $u$ and $v$. For convenience, we define $|G| = |V(G)|$. We will write $P_n$ and $S_n$ for the path and star on $n$ vertices, respectively. A (vertex) coloring $\phi$ is a mapping of $V(G)$ to a set of $k$ colors; we say that $k$ is the size of $\phi$. A color class $C$ of $\phi$ is a maximal set of vertices that for all $u, v \in C$, $\phi(u) = \phi(v)$.

The remainder of this section gives background on subgraph isomorphism counting, bounded expansion, and a related structural class called bounded treedepth.

2.1 Subgraph Isomorphism Counting

Definition 1. Given graphs $G, H$, a subgraph isomorphism from $H$ to $G$ is a mapping $\psi : V(H) \rightarrow V(G)$ such that $uv \in E(H) \iff \psi(u)\psi(v) \in E(G)$.

The subgraph isomorphism counting problem is to count the number of distinct isomorphisms from $V(H)$ to $V(G)$; solving this problem is $\#W[1]$-hard [1, 13].

The most successful algorithms to date used for subgraph isomorphism counting have relied on backtracking [24] or expanding partial mappings [4, 5]. Other subclasses of algorithms have focused on indexing graph databases [21, 11] or creating data structures for parallel computation [23].

Subgraph isomorphism counting is important as a building block for two other network analysis techniques, described below.

Motif Counting: Originally used in the study of cellular biology [22], motif counting computes the number of subgraph isomorphisms expected to occur “by chance” and compares it to the observed subgraph isomorphism count. If $H$ represents some functional unit in the domain of the data—i.e., cliques in social networks corresponding to people with common interests—an unexpected abundance of $H$ in $G$ gives insight into the domain dynamics that caused these motifs to occur.

Graphlet Degree Distribution: Subgraph isomorphism counting is also a building block in the graphlet degree distribution [15], which measures the number of times a vertex occurs in distinct “positions” of multiple small subgraphs. Graphlet degree distributions give a more robust “fingerprint” of a graph’s structure which has in turn been used to uncover underlying domain knowledge [10]. They also have been used in network alignment [15], using the knowledge that two vertices are more likely to be mapped to one another if they occupy the same positions at similar frequencies.

2.2 Bounded Expansion

The algorithms implemented in CONCUSS are designed to exploit bounded expansion network structure. While classes of bounded expansion can be characterized by their $r$-shallow minors [6] or their neighborhood complexities [20], we focus on the algorithmically relevant characterization using $p$-centered colorings.

Definition 2. A $p$-centered coloring of graph $G$ is a vertex coloring such that every connected subgraph $H$ has a unique color or uses at least $p$ colors. The minimum size of a $p$-centered coloring of $G$ is denoted $\chi_p(G)$.

Proposition 2.1. [6] A class of graphs $\mathcal{C}$ has bounded expansion if and only if for some function $f$, every graph $G \in \mathcal{C}$ satisfies $\chi_p(G) \leq f(p)$ for all $p \geq 1$.

Intuitively, $p$-centered colorings identify overlapping, locally well-structured regions of the graph; being in a class of bounded expansion implies the graph can be covered by a small number of such regions. More specifically we note that by Definition 2 for any $p$-centered coloring $\phi$ of graph $G$, if there is a subgraph $H$ for which $\phi_H$ uses fewer than $p$ colors, then every
subgraph of \( H \) has a vertex of unique color. This relates classes of bounded expansion to a much more restricted class of graphs described below.

### 2.3 Centered Colorings and Treedepth

**Definition 3.** A centered coloring of graph \( G \) is a vertex coloring such that every connected subgraph \( H \) has a vertex of unique color, called a center. The minimum number of colors needed for a centered coloring of \( G \) is its centered coloring number, denoted \( \chi_{\text{cen}}(G) \).

Note that a centered coloring is also proper, or else there would be a connected subgraph of size two with no center. Centered colorings are closely related to treedepth decompositions.

**Definition 4.** A treedepth decomposition of a graph \( G \) is an injective mapping \( \psi : V(G) \to V(F) \), where \( F \) is a rooted forest and \( uv \in E(F) \) if \( \psi(u) \) is an ancestor or descendant of \( \psi(v) \). The depth of a treedepth decomposition is the height of \( F \). The treedepth of \( G \), denoted \( \text{td}(G) \), is the minimum depth of a treedepth decomposition of \( G \).

In other words, a treedepth decomposition arranges the vertices of \( G \) in such a way that no edge joins vertices from different branches of the tree.

**Algorithm 1** Treedepth decomposition implied by centered coloring

\[
\phi \leftarrow \text{centered coloring of } G \\
T \leftarrow \text{treedepth decomposition of } G \\
\text{if } |G| = 0 \text{ then return} \\
\text{end if} \\
v \leftarrow \text{center}(\phi | G) \\
\text{root}(T) \leftarrow v \\
\text{for all components } C \in G \setminus \{v\} \text{ do} \\
T' \leftarrow \text{treedepth decomposition of } C \text{ implied by } \phi | C \\
\text{parent(root}(T')) \leftarrow v \\
\text{end for}
\]

Given a centered coloring with \( k \) colors, we can generate a treedepth decomposition of depth at most \( k \) by choosing center \( v \) to be the root and recursing on the components of \( G \setminus \{v\} \), as detailed in Algorithm 1.

In this way, Definition 2 is equivalent to the fact that every small set of colors in a \( p \)-centered coloring induces components with small treedepth.

### 3 CONCUSS

Broadly speaking, the algorithmic pipeline in CONCUSS executes four modules to count the number of isomorphisms of graph \( H \) in \( G \).

1. **COLOR:** Find a \((|H| + 1)\)-centered coloring of \( G \).
2. **DECOMPOSE:** Compute a treedepth decomposition of the subgraph induced by each set of \(|H|\) colors.
3. **COMPUTE:** Using dynamic programming, count the isomorphisms in the treedepth decompositions.
4. **COMBINE:** Combine the counts from previous step to get the total number of isomorphisms in \( G \).

We briefly describe these modules below. Many of the subroutines in the modules can achieve the same high-level functionality with different implementation details, e.g., heuristics, data structures, etc. CONCUSS allows users to specify their choices for some of these subroutines in a configuration file; for more details, see the CONCUSS source code and documentation [17].

These alternatives are designated with teletype.

**Algorithm 2** Sketch of \( p \)-centered coloring

\[
G' \leftarrow G \\
\text{repeat} \\
\text{Orient} \text{ the edges of } G' \text{ to make it a directed acyclic graph of low indegree} \\
\text{Augment } G' \text{ with additional edges based on their orientation} \\
\text{Color} \text{ the vertices greedily} \\
\text{Check} \text{ whether each set of vertices with } p - 1 \text{ colors has low treedepth in } G \\
\text{until} \text{ the coloring is } p\text{-centered}
\]

#### 3.1 Color

The workflow in the COLOR module is outlined in Algorithm 2. The objective is to produce a \( p \)-centered coloring by greedily coloring the vertices of the graph. Because a simple greedy coloring may not immediately be \( p \)-centered, additional edges are added to the graph to impose further constraints. After a bounded number of iterations of the loop in Algorithm 2, a greedy coloring is guaranteed to be \( p \)-centered [6] [19]. Since each substep runs in linear time with respect to \( |G| \), the entire COLOR module also runs in linear time.

*Orient:* The later stages of the COLOR module operate on directed acyclic graphs. In essence, directed edges capture the ancestor relationships in treedepth decompositions of small sets of colors by having edges point from an ancestor to its descendants. In this representation, vertices with large indegree have many ancestors, indicating subgraphs with large treedepth. A low-indegree orientation can be found either with a Degeneracy ordering [14] or by Sandpiling [1].

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Augment: After the edges are oriented, additional directed edges are augmented to the graph to impose more constraints. The placement of the augmenting edges is dependent on the direction of edges in the orientation. Two vertices $a, b$ are said to be transitive if there is some vertex $c$ such that $ac$ and $cb$ are both directed edges in the graph, while $a, b$ are said to be fraternal if there is a vertex $c$ such that $ac$ and $bc$ are both directed edges. The transitive-fraternal augmentation (TFA) algorithm [6] adds the edge $ab$ for every pair of transitive vertices $a, b$ and either the edge $xy$ or $yx$ for every pair of fraternal vertices $x, y$. The orientation of edges between fraternal vertices is chosen to preserve acyclicity and minimize indegree. Distance-truncated transitive fraternal augmentation (DTFA) [19] works similarly, but only requires that some transitive and fraternal edges are added. If $ac$ was added in the $i$th iteration of the loop in Algorithm 2 and $cb$ was added in the $j$th, the edge $ab$ need not be added until the $(i + j + 1)$th iteration.

Color: The acyclic orientation of the edges defines an ordering over which to greedily color the vertices. To minimize the number of colors, CONCUSS uses one of three different heuristics: prioritizing high-degree vertices (High-degree), prioritizing low-degree vertices (Low-degree), or prioritizing vertices with many colors already represented among their neighbors (DSATUR) [2].

Check: Finally, we check whether the coloring is $p$-centered by testing whether each connected subgraph that uses $p - 1$ or fewer colors has a unique color. This can be done by keeping track of components and their respective color multiplicities using union-find structures; when two components merge, we ensure that there is still a unique color. We perform this check at every iteration in order to prevent the algorithm from adding any more colors than necessary.

Other Optimizations: We include additional pre- and post-processing steps to obtain smaller colorings. Vertices of high degree can cause many additional edges to be augmented at each iteration of the loop, which in turn causes more colors to be used. For this reason, removing all high-degree vertices, e.g., degree at least $\sqrt{n}$, finding a coloring of the smaller graph, and then giving each removed vertex a new unique color can reduce the total number of colors. Likewise, in any component of size larger than two, vertices of degree one can be removed and all given the same color in post-processing. After obtaining a $p$-centered coloring, we can also potentially reduce the number of colors by randomly adding transitive and fraternal edges, computing a new greedy coloring, and seeing if this greedy coloring is $p$-centered. The final post-processing step is to check whether pairs of color classes can be merged without violating the $p$-centered property.

3.2 Decompose After the coloring is computed, CONCUSS finds the components induced by each set of $|H|$ colors. To save computation, CONCUSS processes overlapping color sets sequentially in a depth-first search manner. For example, if $|H| = 4$ and 9 colors, the sets would be processed as such: $\{1, 2, 3\}, \{1, 2, 3, 4\}, \{1, 2, 3, 5\}, \ldots, \{1, 2, 3, 9\}, \{1, 2, 4\}, \{1, 2, 4, 5\}, \ldots$.

Given a component induced by a particular color set, a treedepth decomposition is created using Algorithm 1. In order to save memory, these treedepth decompositions are fed into the subsequent Count and Compute stages before a new color set is processed.

3.3 Compute The Compute module uses the dynamic programming algorithm of Demaine et al. [7] to count the isomorphisms of $H$ in a treedepth decomposition. It has exponential time dependence on the small treedepth, but runs in linear time with respect to $|G|$. Briefly, this algorithm exploits the fact that no edges in the treedepth decomposition join vertices in different branches. Therefore, partial pieces of $H$ in one subtree have limited ways of interacting with those in other subtrees. By tracking which pieces occur in each subtree, these counts of partial pieces can be combined to count all isomorphisms in the decomposition.

Integral to the dynamic programming are $k$-patterns, also called boundaried graphs. These (sub)graphs have a subset of vertices labeled uniquely with integers on the interval $[1, k]$, which in turn determine how partial pieces of $H$ can “glue” together.

3.4 Combine The goal in the Combine module is to sum the counts from each treedepth decomposition to get the count for the whole graph. However, because the color sets contain overlapping subgraphs, a simple summation of counts may count some isomorphisms more than once. For example, if $H = P_4$, the subgraph in Figure 3 will be counted in the color sets $\{\text{blue}, \text{orange}, \text{purple}, \text{yellow}\}$, $\{\text{blue}, \text{orange}, \text{purple}, \text{green}\}$, etc. There are multiple ways to rectify this issue. Inclusion-exclusion simply enumerates all color sets with fewer than $|H|$ colors, counts the isomorphisms in those subgraphs, and then applies the inclusion-exclusion principle to correct the counts appropriately. We can also incorporate the combinations into the dynamic programming itself by ignoring counts of color sets that have already been seen (Hybrid).

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2 Edges present originally in $G$ are considered to have been added in the 0th iteration.
3.5 Extensions to other problems We note that the four-stage algorithmic workflow (COLOR, DECOMPOSE, COMPUTE, COMBINE) can be useful for solving problems other than subgraph isomorphism counting. In particular, this approach is amenable to problems in which local subsolutions can be efficiently computed on graphs of low treedepth and then combined to create a global solution. For such a problem, it is possible to reuse the COLOR and DECOMPOSE modules and simply replace the COMPUTE and COMBINE modules with the appropriate alternatives. Dvořák et al. [9] proved that any problem expressible in first-order logic can be solved in this way, such as finding small dominating sets or small independent sets.

4 Experimental Design

We conducted four experiments, one to answer each question posed in Section 1. The first two (Section 3) identify an “optimal” configuration for CONCUSS and test its scalability against an existing subgraph isomorphism counting algorithm. The other two experiments (Section 4) investigate ways in which properties of the coloring affect downstream computation to guide future theoretical research.

To compare the effects of varying multiple options, we normalize two measures $a, b$ using the difference to sum ratio, i.e., $\frac{a-b}{a+b}$. This ratio will be close to 1 when $a \gg b$ and close to $-1$ when $b \gg a$. When comparing times, a positive ratio indicates $b$ is faster than $a$.

4.1 Data Since the theoretical advantages of the algorithms implemented in CONCUSS rely on exploiting structure, it was necessary to ensure our input graphs belonged to classes of bounded expansion. Consequently, we chose three random graph models which asymptotically almost surely produce classes of bounded expansion [7]: the stochastic block model (SB) [12] and the Chung-Lu model, with households (CLH) and without (CL) [8]. The first two models both exhibit clustering commonly found in real-world networks; the CL model was included as a baseline. For each model, we selected configuration parameters known to produce bounded expansion classes. In the CL and CLH models, we used a degree distribution with exponential decay and household size four; for SB we used

$$
\begin{bmatrix}
.40 & .30 & .20 & .10 \\
.50 & .13 & .05 \\
.35 & .11 \\
.45 \\
\end{bmatrix}
$$

as the probability matrix. For each model, three random instances with 1024 vertices and average degree 6 were generated.

4.2 Hardware The experiments were run on identical machines with four-core, 3.0 GHz Intel Xeon E5 v3 processors with a 10 MB cache and 64 GB of memory (4 × 16 GB). Each run of CONCUSS received dedicated resources to avoid interference from other processes.

5 Competitive Evaluation

We evaluated the practicality of CONCUSS by first testing different configurations against one another before comparing them to an existing algorithm.

5.1 Configuration Testing To measure the run times of various configurations, we created one configuration file for each combination of options described in Sections 3.1 and 3.4. For all possible pairings of random instances and configuration options we ran CONCUSS three times. In each run we counted the number of isomorphisms of $P_4$; the particular motif did not vary because the dynamic programming algorithm has theoretically comparable run time for all motifs of the same size. The metrics of interest in each run were the number of colors used, the total elapsed time, and the time specifically spent in the COLOR module. To compare the performance between two implementations of a subroutine, we did a pairwise comparison between configurations in which all other subroutines were held constant. That is to say, to differentiate between $A_1$ and $A_2$, we would compare $(A_1, B_1, C_1)$ against $(A_2, B_1, C_1)$, $(A_1, B_2, C_1)$ against $(A_2, B_2, C_1)$, etc.

Though there were minor variations across graph models, the effects of the different configuration options (Figure 2) were relatively consistent. Orienting the edges using Sandpiling and Degeneracy led to comparable time and coloring sizes. Surprisingly, using DTFA, which is more prudent in augmenting edges, did not outperform TFA in either time or coloring size. We attribute this result to the fact that the average number of augmentation steps needed to reach a $p$-centered coloring was smaller while using TFA (2.9 vs. 4.8), indicating that it may be worth making “suboptimal” choices for...
the augmentations as long as it leads to a $p$-centered coloring sooner. The Low-degree coloring prioritization generally yielded fewer colors and a shorter run time than High-degree, while the more complicated DSATUR prioritization was somewhere in-between. Taken as a whole, the best coloring routine used Degeneracy orientation, TFA, and Low-degree prioritization.

The general distribution of time spent within the Color module also did not vary much with the coloring configuration (Figure 3). Computing the augmentations and coloring the vertices took a very small fraction of the total run time; upwards of 80% of the time was spent ensuring merging color classes kept the coloring $p$-centered, with the pre-merge optimization consuming most of the rest of the time. Nearly all of the computation in these two post-processing routines is in deciding whether a smaller coloring is indeed $p$-centered. As such, small improvements to the efficiency of checking the treedepth of all color sets would pay large dividends in the overall time.

Although the post-processing reduced the coloring size by at least 50% in 90% of the colorings and the total execution time correlated positively with coloring size (Figure 4), we cannot assess whether those optimizations were a net benefit without extrapolating beyond our observed data. Because the time spent merging is dependent on the coloring size, we believe there is a coloring size threshold below which the post-processing is worthwhile; it would be useful to empirically identify this threshold in future work.

The effects of the configurations on the computation downstream from the coloring (Figure 2) were weaker and more varied. In particular, we note that Low-degree prioritization often led to slower downstream computation, but this was offset by the much faster coloring times.

The only configuration option varied outside of the Color module was the method of correcting double
the behavior of various configurations of CONCUSS.

5.2 Comparison with NXVF2 After determining the behavior of various configurations of CONCUSS, we wanted to assess its performance compared to the NetworkX implementation of the popular VF2 algorithm, which we will refer to as NetworkX. We observed that our hypothesis holds when counting stars in $T_{d,s,\ell}$ for sufficiently large $s$. In particular, CONCUSS has more than a fourteen-fold speed advantage over NXVF2 in counting $S_5$ in $T_{12,16,1}$. We believe the difference in time would diverge even more for counting $S_5$ in $T_{14,16,1}$, but NXVF2 already takes nearly 80 hours in $T_{12,16,1}$.

It is also important to note that when $\ell = 1$, the number of paths does not increase in the same way that the number of stars increases. This is because every path of length at least four must contain multiple tree vertices, of which each vertex is adjacent to at most three. Moreover, $P_n$ has exactly two automorphisms (“forwards” and “backwards”) for every $n$, while $S_n$ has $(n-1)!$ automorphisms (any ordering of the leaves). We observed that there were insufficiently many $P_5$s and $P_8$s in $T_{d,s,1}$ to see the same performance benefits, and NXVF2 was consistently faster than CONCUSS.

As predicted, CONCUSS can outperform NXVF2 when counting in $T_{d,s,\ell}$, which has many more $P_5$s and $P_8$s (Figure 5b). Similar to the results shown in Figure 4, CONCUSS counts $P_5$s faster in all graph sizes, while the advantage in counting $P_8$s is only realized in the largest graphs.
Figure 6: Average difference/sum ratio between CONCUSS and NXVF2 on $T_{d,s,ℓ}$ as a function of $s$, the average number of $P_ℓ$s per tree vertex. Each small plot shows a fixed motif and value of $d$. Negative ratios indicate CONCUSS is faster.

6 Bottleneck Identification

Having identified configurations and graph instances in which CONCUSS outperforms NXVF2, we proceeded to identify bottlenecks in CONCUSS that ought to receive further theoretical consideration. We focused on how changing properties of the output of the COLOR module would influence performance in the other three modules.

6.1 Color Class Distribution

Because a graph may admit many distinct $p$-centered colorings of small size, it is important to know whether two colorings of the same size lead to observable differences in the downstream computation. Though the effects the coloring has on the rest of the pipeline almost certainly depend on complex and subtle interactions, we hypothesized that the distribution of sizes of color classes is an important factor. The intuition behind this hypothesis is that different distributions in sizes will lead to different “shapes” of treedepth decompositions, i.e., one large, wide decomposition vs. many small, thin decompositions. To test it, we created colorings of equal size that have unequal distributions of color class sizes. To vary the distributions of color class sizes, we used three splitting heuristics: max, med, and min, which target the maximum-, median-, and minimum-sized color classes.4 When splitting color classes, we chose a random subset of vertices to move into the new color class; to account for this randomness, we repeated each splitting heuristic three times for each coloring. We ran the DECOMPOSE, COMPUTE, and COMBINE modules of CONCUSS three times for each graph instance and associated new coloring, using Inclusion-Exclusion in the COMBINE module.

3 Color classes with exactly one vertex were ignored for calculating the minimum and median sizes.
We observed (Table 1) that \texttt{max} led to the fastest performance, while \texttt{med} and \texttt{min} had very similar run times. The dynamic programming algorithm counts isomorphisms from the leaves of the treedepth decomposition upwards using two operations: \texttt{forgetting}, which moves from children to their parent, and \texttt{joining} which combines results from “siblings” (vertices with the same parent). Since siblings often belong to the same color class, ensuring that no color class has too many vertices limits the number of children, which in turn limits the number of joins. In Table 1 we report that when using \texttt{max} the average number of joins was 33% lower than when splitting the median or minimum-sized classes. Thus future coloring algorithms should attempt to make the sizes of the color classes more uniform.

| Model | Method | Avg time (s) | Joins | Forgets |
|-------|--------|-------------|-------|---------|
| SB    | max    | 856         | $5.12 \times 10^3$ | $2.00 \times 10^3$ |
| SB    | med    | +19%        | +48%  | +13%    |
| SB    | min    | +20%        | +49%  | +13%    |
| CLH   | max    | 1377        | $7.63 \times 10^3$ | $3.01 \times 10^3$ |
| CLH   | med    | +21%        | +48%  | +4%     |
| CLH   | min    | +21%        | +50%  | +6%     |

Table 1: Average run time and dynamic programming operations used for each color splitting heuristic. The statistics for \texttt{med} and \texttt{min} are reported as percent increases over \texttt{max}.

6.2 Color Set Treedepth The dynamic programming (DP) in the \textsc{Compute} module counts isomorphisms of a subgraph of size $h$ in an arbitrary treedepth decomposition of depth $t$. While this algorithm runs in linear time with respect to the size of the graph, it takes $O(t^h)$ time with respect to $t$. One potential direction for further theoretical improvements to the bounded expansion pipeline is to find alternatives to $p$-centered colorings in which subgraphs with at most $i < p$ colors have treedepth that is small but greater than $i$. Ideally, relaxing treedepth requirement would result in a significant reduction in the size of the coloring without dramatically increasing the time spent in DP in the \textsc{Compute} module. Though we cannot measure the size of a hypothetical coloring, we can evaluate how the time per DP operation increases as we count the same subgraph in larger treedepth decompositions. To do this, we computed a 6-centered coloring, enumerated sets of 3, 4, and 5 colors, and counted the number of isomorphisms of $P_3$ in each set.

The run time of the DP algorithm is only dependent on the treedepth of the decompositions insofar as it increases the number of labellings$^4$ of the ancestors of each vertex. There are $t^3 + 3t^2 + t$ such labellings for a $P_3$, each of which requires a constant number of DP operations, so the amount of time spent counting in one color set should grow proportionally to this function.

![Figure 8: Observed vs. predicted average execution time per operation in the stochastic block graphs.](Image)

Table 2: Average execution time per operation and average depth of vertices in the treedepth decomposition. Rows for treedepth $t$ only include those operations incurred in counting in color sets of exactly $t$ colors.

To compare our observations to the predicted growth of $t^3 + 3t^2 + t$, we assumed that the average time per operation for $t = 3$ aligned correctly with this theoretical time and extrapolated outwards for $t \in \{4, 5\}$. As reported in Figure 5, the observed times grow significantly slower than predicted for all operations. The time spent on each operation is dependent on the depth of the vertex in the treedepth decomposition, but the average depth of vertices does not grow at a one-to-one

$^4$These are the $k$-patterns mentioned in Section 3.3 see [7].
ratio with the treedepth (Table 2). This means that the additional color classes add vertices at many depths of the decomposition, rather that simply increasing the depth of every branch uniformly, and thus we seldom "pay" for the cost of the larger depths. Consequently, we conclude that colorings producing deeper decompositions with fewer colors ought to be a viable strategy for improving the overall speed of CONCUSS.

7 Conclusion
We demonstrated that exploiting bounded expansion structure is a promising methodology for scaling subgraph isomorphism counting to larger classes of sparse graphs. We identified through testing various configurations of CONCUSS that orienting with a degeneracy ordering, augmenting with TFA, coloring low-degree vertices first, and combining counts using the inclusion-exclusion principle led to fast run times and small colorings. On sufficiently sparse graphs with high isomorphism counts, CONCUSS was able to significantly outperform NXVF2. In order to get the bounded expansion pipeline to outperform other methods in a broader set of graphs, it is important to understand in future work whether the large coloring sizes of the random graph models were an artifact of the heuristics used in generating the \( p \)-centered colorings, or whether their asymptotically bounded values are actually large.

Our experiments also identified three areas for future theoretical research. The first is to reduce the time needed to verify a coloring is \( p \)-centered, which would yield large dividends in the Color module. The second is to design \( p \)-centered coloring algorithms that balance the sizes of the color classes, consequently reducing the number of join operations. Finally, our results suggest using colorings that trade fewer colors for larger treedepth per color set could be faster than using \( p \)-centered colorings.

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