Final Report — Optimization of Subgraph Isomorphism Algorithm

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Senior Project II

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Contents

1 Introduction

The goal of this project is to understand and optimize an algorithm for solving the NP-complete problem of subgraph isomorphism.

1.1 Background

An *isomorphism* between two graphs is a mapping from the vertices of one graph, say G, to another graph, say H, such that any two vertices which are adjacent in G are mapped to vertices which are adjacent in H. The subgraph isomorphism problem, in turn, is the problem of determining whether an isomorphism exists between a graph G and any of the subgraphs of a larger search graph, H. The issue that makes the subgraph isomorphism problem so difficult to solve for a particular pair of graphs is cycling through the main graph and expanding each node within the graph and checking if each of the generated subgraphs formed from each node is isomorphic to the control graph.

Fortunately, many attempts exist to solve the subgraph isomorphism problem. Among the earliest of these is the famous *Ullmann Algorithm*, proposed by Julian R. Ullmann in his 1976 paper, *An Algorithm for Subgraph Isomorphism.* He first describes a basic, naive approach to finding a mapping from the vertices of a graph to a subgraph of a larger graph. He goes on to define a "refine" procedure to dramatically reduce the number of possible mappings that must be checked.[6] These will be covered in greater detail in the next section.

The goal of our project was to take this algorithm and improve its performance. Subgraph isomorphism is an expensive problem to solve, and finding multiple possible isomorphisms from one graph to subgraphs of another is even more expensive, so even slight improvements in the algorithm's performance is likely to lead to large performance improvements in any large-scale program which needs to use it often.

1.2 Motivation

Our reasoning for choosing this topic for our project is an apparent lack of especially efficient algorithms for solving the subgraph isomorphism problem. Solutions to the subgraph isomorphism problem are often used to detect similarities in chemical compounds,[6] which may shed light on some of their properties. If this process needs to be done, for example, on a very large database of chemical compounds, or less frequently for several very large compounds, the process may take a very long time to complete. It would be very beneficial to improve the performance of this algorithm, even if only slightly, so that these sorts of use cases can still be handled in a more reasonable amount of time.

1.3 Data Set

The primary graph used to test the algorithm and its performance is an undirected graph consisting of "friends lists" from the social media website, Facebook. Each node of the graph represents a unique user, and, if two nodes are adjacent, then their corresponding users are friends on Facebook.[4]

The graph contains 4,039 nodes and 88,234 edges. The relatively large size of the graph makes it well-suited to use for collection of performance data. As we shall see, the Ullmann algorithm takes a rather long time to complete with a graph of this size, allowing any optimizations and/or parallelizations to be readily apparent.

2 Ullmann Algorithm

2.1 Naive Approach

The paper begins, as many do, with a definition of terms that will be used throughout. We have repeated them here for the sake of clarity later on. We begin by noting that the algorithm models the search for a possible mapping by having all possible mappings as nodes on a tree, on which a depth-first search is performed to find a solution.

The subgraph isomorphism problem is defined as the problem of finding all isomorphisms between a graph $G_\alpha = (V_\alpha, E_\alpha)$ and subgraphs of another graph $G_\beta = (V_\beta, E_\beta)$, with (V_α, E_α) and (V_β, E_β) being the set of vertices and edges of G_α and G_β, respectively. The number of vertices and edges of G_α and G_β, respectively, are (p_α, q_α) and (p_β, q_β).

The *adjacency matrix* for graph G_α, $[a_{ij}]$, is defined by:

$$a_{ij} = \begin{cases} 1 & \text{if } i \neq j \text{ and } i, j \text{ share an edge} \\ 0 & \text{otherwise} \end{cases}$$

The adjacency matrix for graph G_β, $[b_{ij}]$, is defined equivalently.

Notably, we have the $p_\alpha \times p_\beta$ matrix M, which is a binary matrix of assignments (mappings) from V_α to V_β. That is, if m_{ij} is 1, then vertex i in graph G_α could possibly be mapped to vertex j in G_β. Otherwise m_{ij} is 0. M has a few interesting properties as a result, which will soon be apparent.

Finally, we come to d, which is simply algorithm's current depth in the search tree. The algorithm starts at $d = 0$, and terminates when $d = p_\alpha$. The matrix M at a particular depth d is denoted as M_d, with solutions to the working instance of the subgraph isomorphism problem being the set of assignments from V_α to V_β, contained within matrices M_{p_α}. M_0 is generated by the following formula:

$$m_{ij} = \begin{cases} 1 & \text{if degree}(j \in G_\beta) \geq \text{ degree}(i \in G_\alpha) \\ 0 & \text{otherwise} \end{cases}$$

Each step of the computation consists of setting all but one of the values of one of the rows of M to 0, and then checking whether exactly one 1 exists in each row. If it does, we have found an isomorphism, since each vertex of G_α has been mapped to exactly one vertex of G_β. If it does not, then we continue onto another row of M and check again. If we have reached the point where we cannot perform the operation on a row of M without violating the condition that each *column* of M contains at most a single 1 (a vertex of G_β cannot be mapped from multiple vertices of G_α), then we backtrack to a previous version of M and try to change the column that we set to 1 in the current row. After exhausting all columns, we conclude there cannot be an isomorphism, since at least one vertex of G_α cannot be mapped to any vertex of G_β.[6]

2.2 "Refine M" Procedure

In the most basic algorithm, the entire tree is searched, including branches which cannot possibly contain a solution at any depth. This is a large number of M matrices to evaluate, so Ullmann introduces a "refine M" procedure to reduce the number that must be checked by eliminating nodes of the tree which cannot contain a solution.

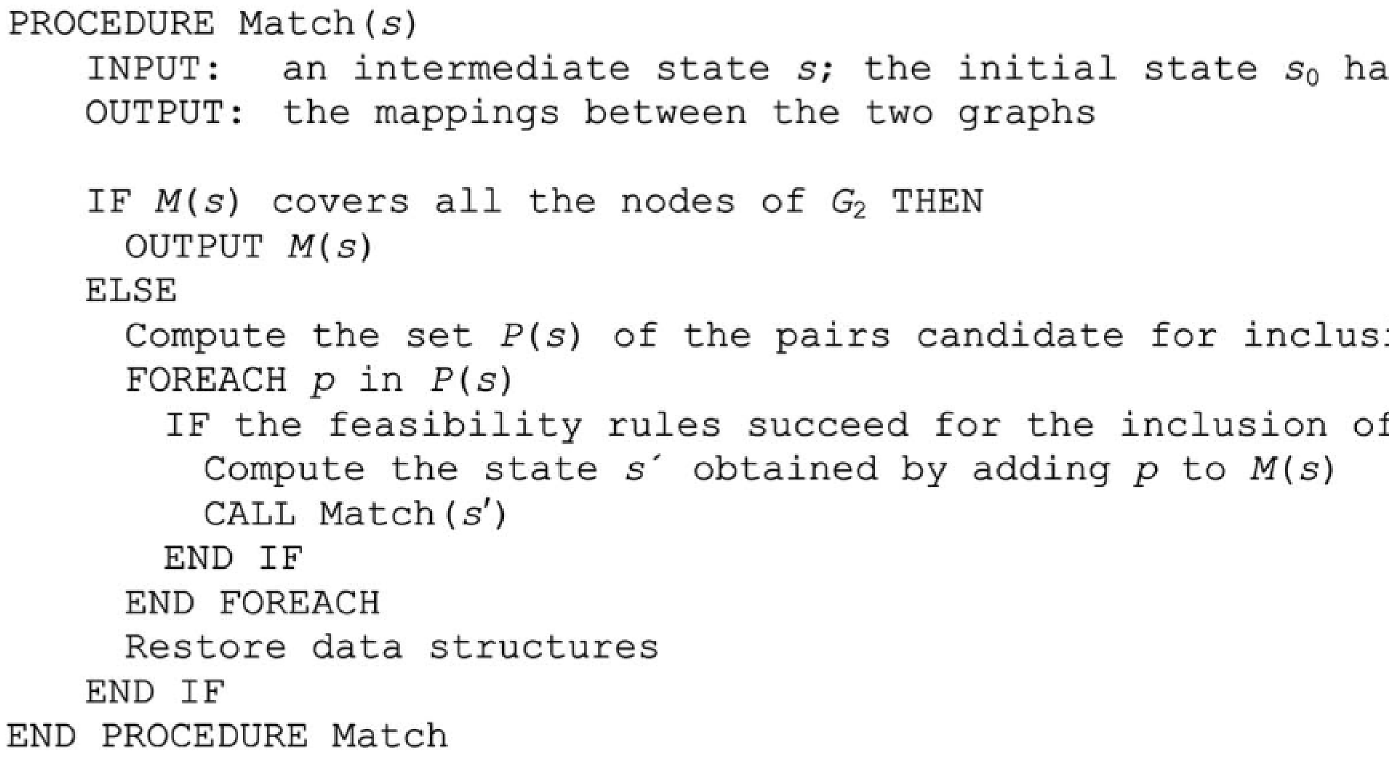
The procedure is actually quite simple. We iterate through each 1 m_{ij} in M and check whether, for each neighbor of the vertex in G_α corresponding to i, there exists at least one possible assignment from it to a neighbor of the vertex in G_β corresponding to j. If this condition does not hold, the 1 is changed to a 0. Since doing so may render other 1s invalid, we repeat the refine procedure on the modified M until running the procedure does not change it any further, indicating that the refinements do not produce any new invalid 1s. This obviously involves several layers of nested loops, adding considerable overhead to the overall algorithm. However, this overhead is very little considering the number of possibilities that are subsequently eliminated, making it a very worthwhile operation to perform regardless.

This refine M procedure is run both on the initial M as well as each of M_d, greatly reducing how many iterations we must perform to see that a particular mapping is invalid.

3 Alternative Algorithms

3.1 VF2 Algorithm

One algorithm that we considered using was the VF2 Algorithm It was developed by Cordella, Foggia, Sansone, and Vento Given two graphs $G1(N_1, B_1)$ and $G2(N_2, B_2)$ and Mapping $M : N_1xN_2$, a subset mapping solution $M(s)$ takes two subgraphs $G_1(s)$ and $G_2(s)$, obtained by selecting from G_1 and G_2 only the nodes included in the components of $M(s)$, and the branches connecting them This is what Cordella's team wrote VF2 to look like



```
PROCEDURE Match($s$)
    INPUT:  an intermediate state $s$; the initial state $s_0$ ha
    OUTPUT: the mappings between the two graphs

    IF $M(s)$ covers all the nodes of $G_2$ THEN
      OUTPUT $M(s)$
    ELSE
      Compute the set $P(s)$ of the pairs candidate for inclus
      FOREACH $p$ in $P(s)$
        IF the feasibility rules succeed for the inclusion of
          Compute the state $s'$ obtained by adding $p$ to $M(s)$
          CALL Match($s'$)
        END IF
      END FOREACH
      Restore data structures
    END IF
END PROCEDURE Match
```

Basically, for each mapping(m, n), it applies five feasibility rules to the current state and the pair to be added Rpred, Rsucc, Rin, Rout, and Rnew. Only if all feasibility rules are satisfied is (n, m) added to the mapping $M(s)$ $F_syn(s, n, m) = R_pred_s^Rucc_i^Rn_o^Rut_n^Rew$ R_pred and R_succ represent the predecessors and successors respectively of a given node n in a graph The other three feasibilty rules are meant to prune the tree R_in and R out are both one step ahead look ahead searches while Rnew is a two step look ahead

These are how each of the feasibility rules are created

$$\begin{aligned}&R_{\text{pred}}(s,n,m) \iff\\&(\forall n' \in M_1(s) \cap \text{Pred}(G_1,n) \exists m' \in \text{Pred}(G_2,m) \mid (n',m') \in M(s)) \wedge\\&(\forall m' \in M_2(s) \cap \text{Pred}(G_2,m) \exists n' \in \text{Pred}(G_1,n) \mid (n',m') \in M(s)),\end{aligned}$$

$$\begin{aligned}&R_{\text{succ}}(s,n,m) \iff\\&(\forall n' \in M_1(s) \cap \text{Succ}(G_1,n) \exists m' \in \text{Succ}(G_2,m) \mid (n',m') \in M(s)) \wedge\\&(\forall m' \in M_2(s) \cap \text{Succ}(G_2,m) \exists n' \in \text{Succ}(G_1,n) \mid (n',m') \in M(s)),\end{aligned}$$

$$\begin{aligned}&R_{\text{in}}(s,n,m) \iff\\&(\text{Card}(\text{Succ}(G_1,n) \cap T_1^{\text{in}}(s)) \geq \text{Card}(\text{Succ}(G_2,m) \cap T_2^{\text{in}}(s))) \wedge\\&(\text{Card}(\text{Pred}(G_1,n) \cap T_1^{\text{in}}(s)) \geq \text{Card}(\text{Pred}(G_2,m) \cap T_2^{\text{in}}(s))),\end{aligned}$$

$$\begin{aligned}&R_{\text{out}}(s,n,m) \iff\\&(\text{Card}(\text{Succ}(G_1,n) \cap T_1^{\text{out}}(s)) \geq \text{Card}(\text{Succ}(G_2,m) \cap T_2^{\text{out}}(s))) \wedge\\&(\text{Card}(\text{Pred}(G_1,n) \cap T_1^{\text{out}}(s)) \geq \text{Card}(\text{Pred}(G_2,m) \cap T_2^{\text{out}}(s))),\end{aligned}$$

$$\begin{aligned}&R_{\text{new}}(s,n,m) \iff\\&\text{Card}(\tilde{N}_1(s) \cap \text{Pred}(G_1,n)) \geq \text{Card}(\tilde{N}_2(s) \cap \text{Pred}(G_2,n)) \wedge\\&\text{Card}(\tilde{N}_1(s) \cap \text{Succ}(G_1,n)) \geq \text{Card}(\tilde{N}_2(s) \cap \text{Succ}(G_2,n)).\end{aligned}$$

In comparison to Ullman's algorithm, it appears that past 200 nodes VF2 becomes more efficient than the Ullman algorithm The time complexity of VF2 is $O(n^2)$ at best and O(N!N) at worst Ullman on the other hand ranges from $O(N^3)$ to $O(N!N^2)$ [3]

3.2 RI Algorithm

For this algorithm, we need to generate all possible maps between two graphs, then check if any of those maps is a subgraph isomorphism.

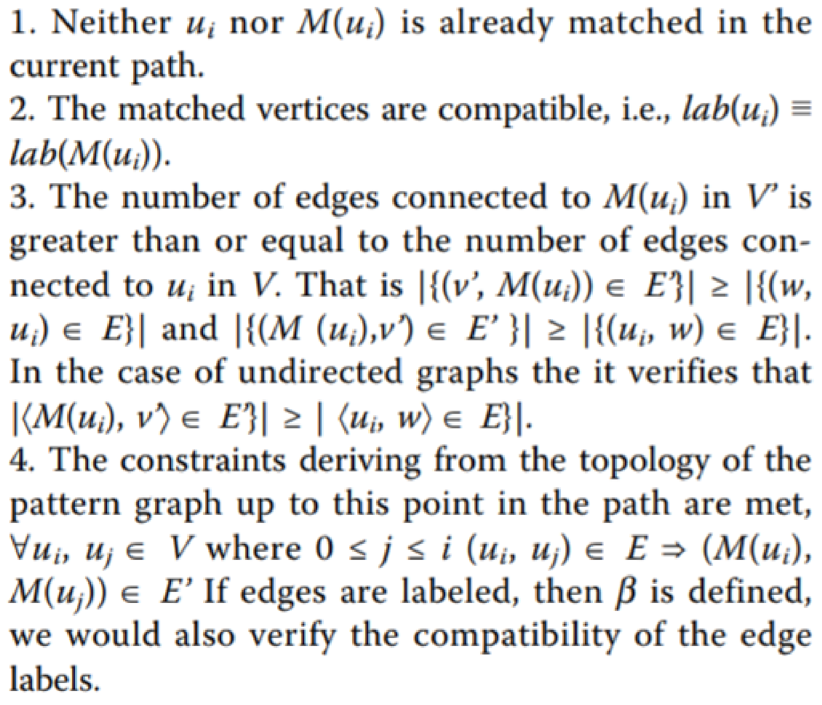
The maps can be represented using a *search space tree*, which has a dummy root. Each node represents a possible match between a vertex in graph G (which is referred to as the pattern graph) in the target graph G'.

Unlike other algorithms, RI orders the vertices of the pattern graph to maximize the chance a partial path will be removed. The idea is to introduce edge constraints as early as possible, and are modeled only on the pattern graph.

RI is also modeled for directed graphs, which allows for more pruning since (u, v) does not imply (v, u) (where u, v are vertices).

The majority of the work is used in a greedy algorithm called /texttt GreatestConstraintFirst, which is used to find a good sequence of vertices based on the number of neighbors a vertex has.

Using the results of `GreatestConstraintFirst`, the following isomorphism rules remove unfeasible paths.



1. Neither u_i nor $M(u_i)$ is already matched in the current path.
2. The matched vertices are compatible, i.e., $lab(u_i) \equiv lab(M(u_i))$.
3. The number of edges connected to $M(u_i)$ in V' is greater than or equal to the number of edges connected to u_i in V. That is $|\{(v', M(u_i)) \in E'\}| \geq |\{(w, u_i) \in E\}|$ and $|\{(M\ (u_i), v') \in E'\ \}| \geq |\{(u_i, w) \in E\}|$. In the case of undirected graphs the it verifies that $|\langle M(u_i), v'\rangle \in E'\}| \geq |\ \langle u_i, w\rangle \in E\}|$.
4. The constraints deriving from the topology of the pattern graph up to this point in the path are met, $\forall u_i, u_j \in\ V$ where $0 \leq j \leq i\ (u_i, u_j) \in\ E \Rightarrow (M(u_i), M(u_j)) \in\ E'$ If edges are labeled, then β is defined, we would also verify the compatibility of the edge labels.

The algorithm does not have a dedicated pruning function, which is another factor for the increase in performance when compared against other algorithms (such as VF2); instead, pruning is done through the matching process.[1]

4 Implementation of the Algorithm

The full source code for all versions can be found in the appendix.

4.1 Python Implementation

The Python code is based largely on an implementation of the Ullmann algorithm provided by an answer on the website *StackOverflow*.[2] It would not run in its original form, so a few adjustments were needed.

```python
def find_isomorphism(graph, subgraph):


    assignments = []
    possible_assignments = [[True]*graph.n_vertices() \
                  for i in range(subgraph.n_vertices())]
    if search(graph, subgraph, assignments, possible_assignments):
        return True
    return matches
```

Listing 1: Function used to determine whether an isomorphism exists.

The main function is `find_isomorphism`, which is depicted above. It calls the function `search`, which performs the actual work of finding an isomorphism.

The `search` function runs the `update_possible_assignments` function. This particular function has been the subject of refining over the course of the project. At the time of the python implementation, it was the most significant bottleneck.

This was mostly due to the usage of the `has_edge` method of the graph class, shown below.

```python
def has_edge(self, vert1, vert2):
     """ Checks if edge connecting vert1 and vert2 is in the graph
     """
     #if adjacent, there's an edge
     return ({vert1, vert2} in self.adjacencies)
```

Listing 2: Code for the `has_edge` method of our graph class.

This method calls the built-in `in` function of Python lists, which has a runtime complexity of O(n).[5] Thus, the `has_edge` method of the Python implementation is O(n).

4.2 Initial C++ Implementation

The initial C++ implementation was based entirely on the Python implementation. Indeed, it represented our best attempt to "translate" the Python code to C++. As one might imagine, it was riddled with compilation errors. That said, we did manage to get it to run, and analysis indicated it performed little better than the Python equivalent. We suspected this was because it retained the same issue that the Python implementation had: calling `has_edge`, an O(n) method, countless times. This motivated a significant improvement.

4.3 Improved C++ Implementation

The improved C++ implementation represents a significant milestone in our project, as it not only improved upon the clarity of the isomorphism algorithm, but also resulted in a much cleaner graph class, with edges implemented as an adjacency matrix. This makes the `has_edge` function O(1), as it consists of simply looking up whether the given vertices share an edge by checking the matrix. This makes its repeated use in `refine_possible_assignments` much more acceptable, a fact which is reflected in the performance.

We also have stored vertices in such a way that each vertex is also stored along with its degree, allowing quick and easy lookup of a vertex's degree.

The improved C++ implementation follows a bit of a loose interpretation of Ullmann's description of the algorithm. A version which used the `goto` command with labels was considered, to more closely match said description, but was scrapped in favor of a more conventional approach

4.4 Optimizations through OpenMP

OpenMP utilizes the multiple cores of a computer's processor in order implement multithreading to run related tasks in parallel. We intend to use it where the bottlenecks in our algorithm are to improve the algorithm's performance. The default number of cores for many computers is four. We intend to place the parallelisms where there tend to be a large number iterations, specifically in loops. This means that, theoretically, the program should run four times faster than without multithreading, using our earlier assumption of four processor cores allotted to the algorithm. It is more likely that it will be approximately 3 to 3.5 times faster, since we may not be able to completely parallelize the bottlenecks as intended. Additionally, using OpenMP, as is the case with any parallelization method, comes with a certain amount of overhead in separating the work to be done. There is also the issue of load balancing: making sure that each thread is performing approximately the same amount of computation so that no thread is idling.

The most important place to place the OpenMP is in the `refine_possible_assignments` function. This function is where the majority of the algorithm's computation takes place, as it has several layers of nested loops, each iterating through vectors which may be very large, depending on the sizes of the graphs being examined. Ideally, we want to balance the loads such that each processor core does an equal amount of work, so as to maximize the amount of parallelization done. However, while we may simply parallelize every iterative process, that might not be efficient enough. Ideally, we would further parallelize in nodes of the search tree which have many possible assignments.

4.5 Sample Run

For visualization purposes, we have provided a sample run of the algorithm. For simplicity, only the C++ implementation is seen here. The graphs used are very simple, as this is only for demonstration. The following is the list of edges defining the search graph:

```
1 2
2 3
```

Listing 3: Search graph used for walkthrough.

And the following is the subgraph we will be searching for an instance of in that graph:

```
10 20
```

Listing 4: Subgraph being searched for in search graph.

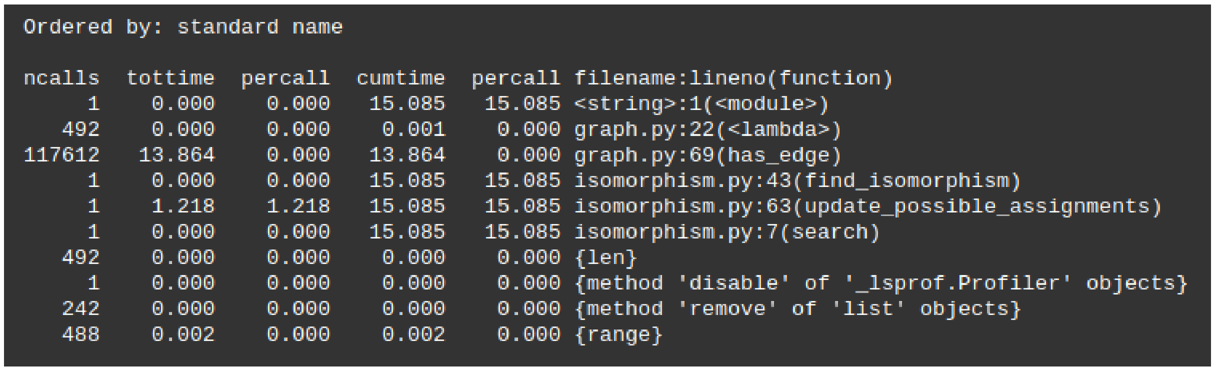
5 Performance

For all of our measurements, we used the worst-case input: the Facebook graph mentioned previously as the search graph, and that same graph (or, equivalently, any isomorphic graph of the same size) as the "subgraph." This would take the longest of the graphs available to us, since it requires the algorithm to assign the greatest number of vertices (all of them) before returning, and, since the graphs are indeed isomorphic, there is no chance of `refine_possible_assignments` returning false, which would allow us to skip a large amount of work.

5.1 Python Implementation

The Python implementation was very inefficient, but it was necessary for us to understand what we had to do for a C++ implementation. It took between 13 and 16 seconds to determine if an isomorphism existed.

We used the Python `cProfile` library to measure the performance of our Python implementation. The documentation is available at `https://docs.python.org/3.5/library/profile.html`. A typical run of the `find_isomorphism` function timed by `cProfile` produces the following output:



```
Ordered by: standard name

ncalls  tottime  percall  cumtime  percall filename:lineno(function)
     1    0.000    0.000   15.085   15.085 <string>:1(<module>)
   492    0.000    0.000    0.001    0.000 graph.py:22(<lambda>)
117612   13.864    0.000   13.864    0.000 graph.py:69(has_edge)
     1    0.000    0.000   15.085   15.085 isomorphism.py:43(find_isomorphism)
     1    1.218    1.218   15.085   15.085 isomorphism.py:63(update_possible_assignments)
     1    0.000    0.000   15.085   15.085 isomorphism.py:7(search)
   492    0.000    0.000    0.000    0.000 {len}
     1    0.000    0.000    0.000    0.000 {method 'disable' of '_lsprof.Profiler' objects}
   242    0.000    0.000    0.000    0.000 {method 'remove' of 'list' objects}
   488    0.002    0.000    0.002    0.000 {range}
```

Figure 1: Sample run of the Python implementation of subgraph isomorphism.

5.2 C++ Implementation

The source code used to test the performance of the C++ implementations can be found in the appendix. We used Linux's `perf_event_open` system call, which allows for high-precision performance monitoring. The only part of the program which is timed is the call to `find_isomorphism`.

The C++ implementation, due to the improvement of `has_edge`'s runtime, runs significantly more quickly than the Python implementation; it runs in about 8 seconds, compared to about 16 seconds for the Python implementation. This is about twice as fast, even without any parallelisms. However, we found it was generally more precise to measure the number of CPU clock cycles taken for the algorithm to complete, so we measured that instead. The output of the program used to measure this is below:

5.3 OpenMP Optimization

The OpenMP code performs very well compared to the non-parallelized version.

6 Conclusion

Over the coming two weeks, we should have completed the OpenMP parallelizations and thoroughly tested the performance of the resulting program. We will also be much more in-depth in the explanation of the Ullmann algorithm. We also hope to use a more precise method of getting performance information for the C++ implementation, as our current method is rather volatile.

7 Appendix

7.1 Python Code

7.1.1 Graph Class

```
"""
Graph module
only has a class
"""
class Vertex:
    """
    Vertex Class
    """
    def __init__(self, label = "", data="", visited=False):
        self.label = label
        self.data = data
        self.visited = visited


class Graph:
    """
    Graph class
    """
    def __init__(self, vertices=None, edges=None, adjacencies=None):
        if vertices is None:
            self.vertices = []
            self.n_vertices = lambda : len(self.vertices)
        else:
            self.vertices = vertices
        if edges is None:
            self.edges = []
        else:
            self.edges = edges
        if adjacencies is None:
            self.adjacencies = []
        else:
            self.adjacencies = adjacencies

        self.__update_adjacencies()

    #Private, don't want anyone calling this by accident.
    def __update_adjacencies(self):
        for edge in self.edges:
            self.adjacencies.append({edge[0], edge[1]})

    def add_vertex(self, vertex=Vertex()):
        """ Add vertex to graph
        """
        self.vertices.append(vertex)

    def remove_vertex(self, vertex):
        """ Remove vertex from graph
            along with edges which contain it
        """
        self.vertices.remove(vertex)
        # list comprehension
        # TLDR remove all elements in self.edges which contain vertex
        # we need this since edges is a list of tuples, not of single elements
        self.edges.remove([edge for edge in self.edges if vertex in edge])
        # see above
        self.adjacencies.remove([adj for adj in self.adjacencies if vertex in adj])

    def add_edge(self, source, dest, weight):
        """ Add edge connecting source and dest
        along with weight
        """
        if (source or dest) not in self.vertices:
            self.vertices.append(source)
            self.vertices.append(dest)

        self.edges.append([source, dest, weight])
        self.adjacencies.append({source, dest})

    def has_edge(self, vert1, vert2):
        """ Checks if edge conecting vert1 and vert2 is in the graph
        """
        #if adjacent, there's an edge
        return ({vert1, vert2} in self.adjacencies)

    # for debugging
    def print_graph(self):
        """ Prints information about the graph
        """
        print("Graph (vertices, edges, adjacencies):")
        print(self.vertices)
        print(self.edges)
        print(self.adjacencies)
```

Listing 5: Python graph class.

7.1.2 Subgraph Isomorphism Algorithm

```
""" Subgraph Isomorphism
CPU Implementation
"""

import copy as cp # for deepcopy
```

```python
def search(graph, subgraph, assignments, possible_assignments):
    """ Uses DFS to find instance of subgraph within larger graph
    """

    update_possible_assignments(graph, subgraph, possible_assignments)

    i = len(assignments)

    # Make sure that every edge between assigned vertices in the subgraph
    # is also an edge in the graph.

    # this loop calls graph.has_edge once for every edge in the subgraph
    for edge in subgraph.edges:
        if edge[0] < i and edge[1] < i:
            if not graph.has_edge(assignments[edge[0]], assignments[edge[1]]):
                return False

    # If all the vertices in the subgraph are assigned, then we are done.
    if i == subgraph.n_vertices():
        return True

    for j in possible_assignments[i]:
        if j not in assignments:
            assignments.append(j)

            # Create a new set of possible assignments, where graph node j
            # is the only possibility for the assignment of subgraph node i.
            new_possible_assignments = cp.deepcopy(possible_assignments)
            new_possible_assignments[i] = [j]

            if search(graph, subgraph, assignments, new_possible_assignments):
                return True
            assignments.pop()

        possible_assignments[i].remove(j)
        update_possible_assignments(graph, subgraph, possible_assignments)

def find_isomorphism(graph, subgraph):

    assignments = []
    possible_assignments = [[True]*graph.n_vertices() \
                            for i in range(subgraph.n_vertices())]
    if search(graph, subgraph, assignments, possible_assignments):
        return True

def update_possible_assignments(graph, subgraph, possible_assignments):
    """ docstring to suppress the warning
    """
    any_changes = True
    while any_changes:
        any_changes = False
        for i in range(0, subgraph.n_vertices()):
            for j in possible_assignments[i]:
                for adj in subgraph.adjacencies(i):
                    match = False
                    for vert in range(0, graph.n_vertices()):
                        # graph.has_edge gets called once
                        # for every vertex in the graph
                        # for every item in the subgraph's adjacencies
                        # for every possible assignments
                        # that is a huge number of calls to has_edge
                        # which is in itself an O(n) operation
                        # definitely room for improvement.
                        if adj in possible_assignments[adj] and \
                                graph.has_edge(j, vert):
                            match = True
                    if not match:
                        possible_assignments[i].remove(j)
                        any_changes = True
```

Listing 6: Python algorithm to find isomorphism.

7.1.3 Main

```
""" Main
"""
import sys #args
import getopt
from graph import Graph
from isomorphism import find_isomorphism
import cProfile

def main(argv):
    """ Main function
    """
    argc = len(argv)

    interactive, debug = handle_args(argc, argv)

    if interactive:
        print("Enter the graph as a space-separated adjacency list of the form\
                node1 node2 [edge_weight]:")
        filename = sys.stdin
    else:
        filename = argv[1]
    graph = import_data(filename, debug)

    if debug:
        graph.print_graph()

    if interactive:
        print("Enter the subgraph using the same format:")
        sub = sys.stdin
    else:
        sub = argv[2]

    subgraph = import_data(sub, debug)

    if debug:
        subgraph.print_graph()

    cProfile.runctx('find_isomorphism(graph, subgraph)', globals(), locals())

def import_data(filename, debug):
    """ Takes graph adjacency list written in file fd
        creates and returns graph object representing
        the graph in the file
        Note that edge weights are all 0 unless otherwise specified.
    """
    if filename == sys.stdin:
        fdesc = filename
    else:
        try:
            fdesc = open(filename, 'r')
        except IOError as err:
            sys.stderr.write("Error: Could not open file '%s'. Aborting.\n%s\n" \
                    % (filename, err))
            sys.exit(2)

    if debug:
        print(fdesc)

    graph = Graph()

    if debug:
        print("Reading file")
    for line in fdesc:
        vals = line.split()
        if len(vals) == 3:
            edge_weight = int(vals[2])
        elif len(vals) > 2:
            sys.stderr.write("Error reading file '%s'. Data should be in form \
                    'node1 node2 [edge_weight]', but line was %s\n" % line)
            sys.exit(3)
        else:
            edge_weight = 0

        graph.add_edge(int(vals[0]), int(vals[1]), edge_weight)

    if filename != sys.stdin:
        fdesc.close()

    return graph

def usage(name, err):
    """ Prints usage info
    """
    usg = """usage: %s [FILE] [OPTION]
    Options and arguments:
```

```
    FILE:                Space-separated file containing graph adjacency list. \
            If edge weights are not specified, all weights will be assumed 0.
    -h, --help:          Print this help message and exit.
    -i, --interactive:   Get space-separated graph adjacency list from stdin.
    -d, --debug:         Print debugging information.\n"""
    if err:
        sys.stderr.write(usg % name)
        return

    sys.stdout.write(usg % name)

def handle_args(argc, argv):
    """ get command line arguments, set variables accordingly
    """
    # TODO change to False for final deployment
    debug = True
    interactive = False

    # arguments should be either 2 files or the two files and some args
    # unless -i is specified in which case just the args
    if argc < 2:
        usage(argv[0], True)
        sys.exit(1)
    else:
        try:
            # using _ as a variable name is sort of the conventional way of saying
            # "we don't need or use this variable but i'm assigning it because
            # the method or api or whatever i'm using requires it"
            _, args = getopt.getopt(argv, "hid", ["help", "interactive", "debug"])
        except getopt.GetoptError:
            # print usage info and quit
            usage(argv[0], True)
            sys.exit(1)
        # handle args
        for arg in args:
            if arg in ("-h", "--help"):
                usage(argv[0], False)
                sys.exit()
            elif arg in ("-i", "--interactive"):
                interactive = True
                args.remove(arg)
            elif arg in ("-d", "--debug"):
                debug = True
                args.remove(arg)

    return interactive, debug


if __name__ == "__main__":
    main(sys.argv)
```

Listing 7: Python main function to process arguments and run the ismorphism algorithm.

7.2 C++ Code

7.2.1 Graph Class

```
#include <algorithm> //Replace, remove, find
#include <iostream>
#include "graph.h"


using std::remove;
using std::find;
using std::get;
using std::cout;
using std::map;
using std::unordered_set;
```

```
struct CompareFirst
{
  CompareFirst(int val) : val_(val) {}
  bool operator()(const std::pair<int,int>& elem) const {
    return val_ == elem.first;
  }
  private:
    int val_;
};

// edges[i][j] = weight of edge connecting i and j
// -1 if no such edge

Graph::Graph () {
  this->vertices = vector<pair<int, int> >();
  this->edges = vector<vector<int> >();
  this->adjacencies = vector<unordered_set<int> >();
  this->vertex_indices = map<int, int>();
  this->vertex_vals = map<int, int>();
}

void Graph::add_vertex(pair<int, int> vertex) {
  if (this->get_index(vertex.first) < 0) {
    this->vertices.push_back(vertex);
    // add mappings
    //vertex_indices[vertex.first] = vertices.size()-1;
    this->vertex_indices.insert(pair<int, int>(vertex.first, vertices.size()-1));

    //vertex_vals[vertices.size()-1] = vertex.first;
    this->vertex_vals.insert(pair<int, int>(vertices.size()-1, vertex.first));
    // add row with edges.size()+1 -1s
    this->edges.push_back(vector<int>(edges.size()+1,-1));
    // add a set for its neighbors
    this->adjacencies.push_back(unordered_set<int>());
  }
}

void Graph::add_edge(int source, int dest, int weight) {

  // WEIGHT SHOULD BE NON-NEGATIVE
  this->add_vertex(pair<int, int>(source, 0));

  this->add_vertex(pair<int, int>(dest, 0));

  int sourceind = this->get_index(source);
  int destind = this->get_index(dest);

  // increase vertex degree
  this->vertices[this->get_index(source)].second++;
  this->vertices[this->get_index(dest)].second++;

  // source -> dest
  if (sourceind < destind) {
    this->edges[destind][sourceind] = weight;
  }

  else {
    this->edges[sourceind][destind] = weight;
  }
  // TODO: get adjacency set of source and dest (or create them if not in graph)
  // add dest/source to that set
  // once again, consider directed graphs
  this->add_neighbor(source, dest);
  this->add_neighbor(dest, source);
}

bool Graph::has_edge(int vert1, int vert2){
  // just got this bad boy down to O(1)
  // you're welcome
  return (edges[vert1][vert2] >= 0);
}

int Graph::get_index(int value) {
  if (this->vertex_indices.find(value) != this->vertex_indices.end()) {
    return this->vertex_indices[value];
  }

  return -1;
}

int Graph::get_value(int index) {
  if (this->vertex_vals.find(index) != this->vertex_vals.end()) {
    return this->vertex_vals[index];
  }

  return -1;
}



unordered_set<int> Graph::neighbors(int vertex) {
  return this->adjacencies[this->get_index(vertex)];
}

void Graph::add_neighbor (int vert, int neighbor) {
  this->neighbors(vert).insert(this->vertices[this->get_index(neighbor)].first);
}

// basically obselete now
//void Graph::update_adjacencies() {
//   for (size_t i = 0; i < edges.size(); i++){
//     unordered_set<int> edge ({get<0>(edges[i]), get<1>(edges[i])});
//     adjacencies.push_back(edge);
//   }
//}

// void Graph::print_graph() {
//    cout << "Begin graph" << std::endl;
//    cout << "--------------------------------\n";
//    cout << "Vertices: " << vertices << std::endl;
//    cout << "Edges: " << edges << std::endl;
//    cout << "--------------------------------\n";
//    cout << "End graph" << std::endl;
// }
```

Listing 8: C++ graph class.

7.2.2 Subgraph Isomorphism Algorithm

```
#include <vector>
#include <utility>
#include <unordered_set>
#include <algorithm> //for std::find
#include "isomorphism.h"

using std::find;

vector <int> find_isomorphism (Graph &sub, Graph &graph) {
```

```
vector < vector<bool> > possible_assignments = create_possible_assignments(sub, graph);
vector <vector <vector <bool> > > assignments_tree;
// we need a way to keep track of which columns we've already assigned for each row
// cols_used[i] == true if column i has already been used
vector <bool> cols_used = vector<bool>(possible_assignments[0].size(), false);
// keep track of which column was used at which depth
// col_depth[i-1] == k iff column k was used at depth i
vector <size_t> col_depth = vector<size_t>(possible_assignments.size(), 0);

size_t depth = 1;

if (search(sub, graph, assignments_tree, possible_assignments, cols_used, col_depth, dept

  vector<vector<bool> > assignments = assignments_tree[depth-2];
  vector<int> isomorphism;
  for (size_t i = 0; i < assignments.size(); i++) {
    //fprintf(stderr, "Row %lu\n", i);
    for (size_t j = 0; j < assignments[i].size(); j++) {
      //fprintf(stderr, "%d\n", assignments[i][j] ? 1 : 0);
      if (assignments[i][j]) {
        isomorphism.push_back(j);
        // go to next row
        // no need to waste iterations
        break;
      }
    }
  }

  return isomorphism;
}
```

```
  return vector<int>(0);
}

bool search (Graph &sub, Graph &graph,
      vector<vector<vector<bool> > > &assignments_tree,
      vector<vector<bool> > &possible_assignments,
      vector<bool> &cols_used,
      vector<size_t> &col_depth,
      size_t &depth) {

  // if refine fails, no possible isomorphism
  if (!refine_possible_assignments(sub, graph, possible_assignments)) {
    return false;
  }

  do {
    size_t numrows = possible_assignments.size(), numcols = possible_assignments[0].size()

    for (col = col_depth[depth-1]; col < numcols; col++) {
      // find first column we havent already used
      // col is index of vertex in search graph we're trying to assign
      // we start searching from col_depth[depth-1]+1 since
      // that's the col after the one we attempted previously and
      // we gotta find the next one
      if (possible_assignments[depth-1][col] && !cols_used[col]) {
        break;
      }
    }

    if (col == numcols) {
      // we couldn't find a valid column.
      // if we're on depth 1, there's no level to go back up to
      // no possible isomorphism
      if (depth == 1) {
        return false;
      }

      // otherwise, go up to the previous depth and try to assign that
      // row to another column
      else {
        depth--;
        possible_assignments = assignments_tree[depth-1];
        return false;
      }
    }

    // we found a valid column
    // set all other possible assignments in this col to 0
    // if we're assigning this vertex to the subgraph vertex
    // we can't have any other subgraph vertex also assigned to it
    size_t i;
    for (i = 0; i < numrows; i++) {
      if (i != depth-1) {
        possible_assignments[i][col] = false;
      }
    }

    // set all other 1s in this row to 0
    // we can only assign each subgraph vertex to a single column
    for (i = 0; i < numcols; i++) {
      if (i != col) {
        possible_assignments[depth-1][i] = false;
      }
    }
    // now go to the next row and repeat
    // we used this column
    cols_used[col] = true;
    // and we used it at this depth
    col_depth[depth-1] = col;
    // save a copy of possible assignments
    assignments_tree.push_back(possible_assignments);
    // increment depth
    depth++;

    if (depth == possible_assignments.size()) {
      // we've assigned every row to a column
      // isomorphism found
      return true;
    }

    // if we get all the way to the bottom by doing this repeatedly,
    // we'll have found an isomorphism
    if (search(sub, graph, assignments_tree, possible_assignments, cols_used, col_depth, de
      return true;
    }
    else {
      // that didn't work. find a new column.
      cols_used[col] = false;
    }
    // this is fine since we only get here if we need to find a new column
  } while (true);
}

vector < vector<bool> > create_possible_assignments(Graph &sub, Graph &graph) {
  // possible_assignments[i][j] == true iff a possible assignment exists from i in sub
  // to j in search graph
  vector < vector<bool> > possible_assignments (sub.vertices.size(),
    vector<bool>(graph.vertices.size(), false));

  // at first, every vertex in search graph with rank >= i is a possible assignment
  // this will be refined later
  // see refine_possible_assignments
  size_t i, j;
  size_t s_n = sub.vertices.size();
  size_t g_n = graph.vertices.size();
  for (i = 0; i < s_n; i++) {
    for (j = 0; j < g_n; j++) {
      if (graph.vertices[j].second >= sub.vertices[i].second) {
        possible_assignments[i][j] = true;
      }
    }
  }

  return possible_assignments;
}

bool refine_possible_assignments(Graph &sub, Graph &graph, vector < vector<bool> > &possib
  size_t i, j;
  size_t pa_n = possible_assignments.size();
  size_t pb_n = possible_assignments[0].size();
  bool changes_made = true;

  while (changes_made) {
    changes_made = false;
    for (i = 0; i < pa_n; i++) {
      // check if this row contains no 1s
      bool no_one = true;
```

```
for (j = 0; j < pb_n; j++) {
  if (possible_assignments[i][j]) {
    no_one = false;
    // check if all of i's neighbors have a possible assignment to a neighbor of j
    // iterate through all neighbors of i
    unordered_set<int> neighbors_i = sub.neighbors(sub.get_value(i));
    unordered_set<int>::iterator n_i = neighbors_i.begin();

    for (; n_i != neighbors_i.end(); n_i++) {
      // for each neighbor of i, iterate through all its possible assignments
      size_t k;
      bool has_corresponding_neighbor = false;
      for (k = 0; k < pb_n; k++) {
        if (possible_assignments[sub.get_index(*(n_i))][k]) {
          // for each possible assignment from i's neighbor to graph, check if it is
          if (graph.has_edge(graph.get_value(j), graph.get_value(k))) {
            // if so, then check the next neighbor
            has_corresponding_neighbor = true;
            break;
          }
        }
      }

      // if this neighbor has no corresponding neighbor, then j is an invalid match.
      // move on to the next possible assignment
      if (!has_corresponding_neighbor) {
        possible_assignments[i][j] = 0;
        changes_made = true;
        break;
      }
    }
  }
```

```
      }

      // we never found a 1 in this row, so there's no point in continuing
      // there's at least one vertex in subgraph that cannot be mapped to any
      // vertex in the search graph, so we know that
      // possible_assignments cannot specify any isomorphism
      if (no_one) {
        return false;
      }
    }
  }

  // M was successfully refined without creating any rows with all 0s. return true.
  return true;
}
```

Listing 9: C++ algorithm to find isomorphism.

7.2.3 Main

```
// use stderr to print debug info since stderr is unbuffered
// i.e. anything sent to stderr will be printed immediately
// instead of put into a buffer and printed when the buffer
// gets flushed
#include <cstdio>
#include <cstdlib>
#include <cstring>
#include <iostream> //debugging
#include <vector>
#include <tuple>
#include <getopt.h>
#include <sys/types.h>
#include <sys/stat.h>
```

```
#include <unistd.h>
#include <fcntl.h>
#include <errno.h>
#include "graph.h"
#include "isomorphism.h"
#include <unordered_set>
#include <cstring>
using std::string;

const char* program_name;

vector<string> handle_args(int argc, char **argv);
void usage (FILE* stream, int exit_code);
Graph import_data(const char *filename, const int debug);

int main(int argc, char **argv) {

  program_name = argv[0];

  vector<string> args = handle_args(argc, argv);

  int interactive = atoi(args[0].c_str());
  int debug = atoi(args[1].c_str());

  char filename_default[] = "stdin";

  const char *graph_filename = (!interactive) ? args[2].c_str()
                                              : filename_default;
  const char *sub_filename = (!interactive) ? args[3].c_str()
                                              : filename_default;

  if (debug) {
    fprintf(stderr, "inter = %d, debug = %d\n", interactive, debug);
    fprintf(stderr, "Graph file %s, subgraph file %s\n", graph_filename, sub_filename);
  }


  Graph graph = import_data(graph_filename, debug);

  if (debug) {
    fprintf(stderr, "Successfully imported graph from file %s.\n",
        graph_filename);
  }

  Graph subgraph = import_data(sub_filename, debug);

  if (debug) {
    fprintf(stderr, "Successfully imported subgraph from file %s.\n",
        sub_filename);
  }

  if (debug) {
    fprintf(stderr, "Running find_isomorphism....\n");
  }

  vector<int> isomorphism = find_isomorphism(subgraph, graph);

  if (debug){
    fprintf(stderr, "find_isomorphism terminated.\n");
  }

  if (isomorphism.size() == 0) {
    printf("No isomorphism found.\n");
  }
  else{
    printf("Isomorphism found! Assignments are:\n");
    size_t num_assignments = isomorphism.size();
    for (size_t i = 0; i < num_assignments; i++) {
      int subgraph_vert = subgraph.get_value(i);
      int graph_vert = graph.get_value(isomorphism[i]);
      printf("Vertex %d maps to vertex %d\n", subgraph_vert, graph_vert);
    }
  }

  return 0;
}

Graph import_data(const char *filename, const int debug) {

  FILE *fd;
  if (strcmp(filename, "stdin") == 0) {
    fd = stdin;
  }

  else {
    fd = fopen(filename, "r");
    if (fd == NULL) {
      fprintf(stderr, "Could not open file %s for reading.\n", filename);
      perror("Error calling fopen()");
      exit(errno);
    }
  }

  char *line = NULL;
  size_t n = 0;
```

```
Graph g;

if (debug) {
  fprintf(stderr, "Reading file %s...\n", filename);
}

char *tempa, *tempb, *tempweight;
char tempweight_default[] = "0";
ssize_t bytes_read;
// getline returns -1 on failure to read a line (including EOF)
bytes_read = getline(&line, &n, fd);
while (bytes_read != -1) {
  tempa = strtok(line, " ");
  // strtok returns NULL if the token (space in this case) was not found in the str
  // otherwise return the string up to the token (exclusive)
  if (tempa == NULL) {
    fprintf(stderr, "Error parsing file %s. Adjacency list must be of form 'node1 node2
        but line was %s\n", filename, line);
    exit(-1);
  }

  // if arg is null after a call to strtok, it'll keep reading after the position of the
  tempb = strtok(NULL, " ");
  if (tempb == NULL) {
    fprintf(stderr, "Error parsing file %s. Adjacency list must be of form 'node1 node2
        but line was %s\n", filename, line);
    exit(-1);
  }

  tempweight = strtok(NULL, " ");
  if (tempweight == NULL) {
      tempweight = tempweight_default;
    }

    int atempa = atoi(tempa);
    int atempb = atoi(tempb);
    int atempweight = atoi(tempweight);

    //printf("Edge is %d %d %d\n", atempa, atempb, atempweight);
    // this will also add the vertices if they don't exist
    // add_vertex is called from within add_edge if no vertex with the given value exists
    g.add_edge(atempa, atempb, atempweight);
    bytes_read = getline(&line, &n, fd);
  }

  if (fd != stdin) {
    int stat = fclose(fd);
    if (stat != 0) {
      perror("Error closing file");
      // we never wrote to the file so we probably don't even need to check for errors in t
      // but just kill the program if there's an error closing it
      exit(errno);
    }
  }

  // don't free line since it's null now

  return g;
}

vector<string> handle_args(int argc, char **argv) {
  // for getopt
  const char* const short_options = "hid";
  const struct option long_options[] = {
    { "help",  0, NULL, 'h' },
    { "interactive", 0, NULL, 'i'},
    { "debug", 0, NULL, 'd'},
    { NULL, 0, NULL, 0 }
  };

  vector<string> returnargs;
  returnargs.resize(4);
  int interactive = 0;
  // TODO change to 0 for final deployment
  int debug = 1;

  if (argc < 2) {
    usage(stderr, 1);
  }

  int next_option;
  do {
    next_option = getopt_long(argc, argv, short_options,
                              long_options, NULL);
    switch(next_option) {
      case 'h':
        usage(stdout, 0);
        // calling usage quits the program anyway but whatever
        // we'll put a break here anyway
        break;

      case 'i':
        interactive = 1;
        break;
      case 'd':
        debug = 1;
        break;

      case '?': // invalid option
        usage(stderr, 1);
        break;

      case -1: // no more options
        break;

      default: // something went very wrong if we got here
        abort();
    }
  }
  while (next_option != -1);

  // now that we've gone through all the options, OPIND points to first
  // nonoption argument. which is hopefully the first filename. unless
  // interactive was specified, in which case yell at the user.

  if (!interactive) {
    returnargs[2] = string(argv[optind]);
    returnargs[3] = string(argv[optind+1]);

  }

  if (debug) {
    fprintf(stderr,"Interactive set to %d. Debug is %d.\n", interactive, debug);
    if (!interactive) {
      fprintf(stderr,"Using file %s for graph and %s for subgraph.\n",argv[optind],argv[opt
    }
  }

  // put what we want to return in their places.
  returnargs[0] = std::to_string(interactive);
  returnargs[1] = std::to_string(debug);

  return returnargs;
}

void usage (FILE* stream, int exit_code) {
  fprintf(stream, "usage: %s [FILE] [OPTION]\n", program_name);
  fprintf(stream,
    "Options and arguments:\n"
    "FILE:                 Space-separated file containing graph adjacency list. If edge wei
    "-h, --help:           Print this help message and exit.\n"
    "-i, --interactive:    Get space-separated graph adjacency list from stdin.\n"
    "-d, --debug:          Print debugging information.\n");

  exit(exit_code);
}
```

Listing 10: C++ main function to process arguments and run the ismorphism algorithm.

7.3 OpenMP Code

Note: Since the OpenMP version of our algorithm uses the same graph class and `main.cpp`, we have omitted them from this section.

7.3.1 Subgraph Isomorphism Algorithm

```
#include <vector>
#include <utility>
#include <unordered_set>
#include <algorithm> //for std::find
```

```
#include "isomorphism.h"
#include "omp.h"

int THREADS = omp_get_max_threads();

using std::find;

vector <int> find_isomorphism (Graph &sub, Graph &graph) {

  vector < vector<bool> > possible_assignments = create_possible_assignments(sub, graph);
  vector <vector <vector <bool> > > assignments_tree;
  // we need a way to keep track of which columns we've already assigned for each row
  // cols_used[i] == true if column i has already been used
  vector <bool> cols_used = vector<bool>(possible_assignments[0].size(), false);
  // keep track of which column was used at which depth
  // col_depth[i-1] == k iff column k was used at depth i
  vector <size_t> col_depth = vector<size_t>(possible_assignments.size(), 0);

  size_t depth = 1;

  if (search(sub, graph, assignments_tree, possible_assignments, cols_used, col_depth, dept

    vector<vector<bool> > assignments = assignments_tree[depth-2];
    vector<int> isomorphism;
    for (size_t i = 0; i < assignments.size(); i++) {
      //fprintf(stderr, "Row %lu\n", i);
      for (size_t j = 0; j < assignments[i].size(); j++) {
        //fprintf(stderr, "%d\n", assignments[i][j] ? 1 : 0);
        if (assignments[i][j]) {
          isomorphism.push_back(j);
          // go to next row
          // no need to waste iterations
          break;
        }
      }
    }

    return isomorphism;
  }

  return vector<int>(0);
}

bool search (Graph &sub, Graph &graph,
      vector<vector<vector<bool> > > &assignments_tree,
      vector<vector<bool> > &possible_assignments,
      vector<bool> &cols_used,
      vector<size_t> &col_depth,
      size_t &depth) {

  // if refine fails, no possible isomorphism
  if (!refine_possible_assignments(sub, graph, possible_assignments)) {
    return false;
  }

  do {
    size_t numrows = possible_assignments.size(), numcols = possible_assignments[0].size()

    for (col = col_depth[depth-1]; col < numcols; col++) {
      // find first column we havent already used
      // col is index of vertex in search graph we're trying to assign
      // we start searching from col_depth[depth-1]+1 since
      // that's the col after the one we attempted previously and
      // we gotta find the next one
      if (possible_assignments[depth-1][col] && !cols_used[col]) {
        break;
      }
    }

    if (col == numcols) {
      // we couldn't find a valid column.
      // if we're on depth 1, there's no level to go back up to
      // no possible isomorphism
      if (depth == 1) {
        return false;
      }

      // otherwise, go up to the previous depth and try to assign that
      // row to another column
      else {
        depth--;
        possible_assignments = assignments_tree[depth-1];
        return false;
      }
    }

    // we found a valid column
    // set all other possible assignments in this col to 0
    // if we're assigning this vertex to the subgraph vertex
    // we can't have any other subgraph vertex also assigned to it
    size_t i;
    for (i = 0; i < numrows; i++) {
      if (i != depth-1) {
        possible_assignments[i][col] = false;
      }
    }
```

```
// set all other 1s in this row to 0
// we can only assign each subgraph vertex to a single column
for (i = 0; i < numcols; i++) {
  if (i != col) {
    possible_assignments[depth-1][i] = false;
  }
}

// now go to the next row and repeat
// we used this column
cols_used[col] = true;
// and we used it at this depth
col_depth[depth-1] = col;
// save a copy of possible assignments
assignments_tree.push_back(possible_assignments);
// increment depth
depth++;

if (depth == possible_assignments.size()) {
  // we've assigned every row to a column
  // isomorphism found
  return true;
}

// if we get all the way to the bottom by doing this repeatedly,
// we'll have found an isomorphism
if (search(sub, graph, assignments_tree, possible_assignments, cols_used, col_depth, de
  return true;
}
else {
  // that didn't work. find a new column.
```

```
      cols_used[col] = false;
    }
    // this is fine since we only get here if we need to find a new column
  } while (true);
}

vector < vector<bool> > create_possible_assignments(Graph &sub, Graph &graph) {
  // possible_assignments[i][j] == true iff a possible assignment exists from i in sub
  // to j in search graph
  vector < vector<bool> > possible_assignments (sub.vertices.size(),
    vector<bool>(graph.vertices.size(), false));

  // at first, every vertex in search graph with rank >= i is a possible assignment
  // this will be refined later
  // see refine_possible_assignments
  size_t i, j;
  size_t s_n = sub.vertices.size();
  size_t g_n = graph.vertices.size();
  for (i = 0; i < s_n; i++) {
    for (j = 0; j < g_n; j++) {
      if (graph.vertices[j].second >= sub.vertices[i].second) {
        possible_assignments[i][j] = true;
      }
    }
  }

  return possible_assignments;
}

bool refine_possible_assignments(Graph &sub, Graph &graph, vector < vector<bool> > &possibl
  size_t i, j;
  size_t pa_n = possible_assignments.size();
  size_t pb_n = possible_assignments[0].size();
  bool changes_made = true;

  while (changes_made) {
    changes_made = false;
    bool no_one = true;
    for (i = 0; i < pa_n; i++) {
      // check if this row contains no 1s
      no_one = true;
    #pragma omp parallel num_threads(THREADS)
      for (j = 0; j < pb_n; j++) {
        if (possible_assignments[i][j]) {
          no_one = false;
          // check if all of i's neighbors have a possible assignment to a neighbor of j
          // iterate through all neighbors of i
          unordered_set<int> neighbors_i = sub.neighbors(sub.get_value(i));
          unordered_set<int>::iterator n_i = neighbors_i.begin();

          for (; n_i != neighbors_i.end(); n_i++) {
            // for each neighbor of i, iterate through all its possible assignments
            size_t k;
            bool has_corresponding_neighbor = false;
            for (k = 0; k < pb_n; k++) {
              if (possible_assignments[sub.get_index(*(n_i))][k]) {
                // for each possible assignment from i's neighbor to graph, check if it is
                if (graph.has_edge(graph.get_value(j), graph.get_value(k))) {
                  // if so, then check the next neighbor
                  has_corresponding_neighbor = true;
                  break;
                }
              }
            }
```

```
            // if this neighbor has no corresponding neighbor, then j is an invalid match.
            // move on to the next possible assignment
            if (!has_corresponding_neighbor) {
              possible_assignments[i][j] = 0;
              changes_made = true;
              break;
            }
          }
        }
      }

      // we never found a 1 in this row, so there's no point in continuing
      // there's at least one vertex in subgraph that cannot be mapped to any
      // vertex in the search graph, so we know that
      // possible_assignments cannot specify any isomorphism
      if (no_one) {
        return false;
      }
    }
  }

  // M was successfully refined without creating any rows with all 0s. return true.
  return true;
}
```

Listing 11: C++ algorithm to find isomorphism, with parallelisms through OpenMP.

7.4 Code Used to Check Performance of C++ code

```
#include <cstdio>
#include <cstdlib>
#include <cstring>
```

```
#include <getopt.h>
#include <sys/types.h>
#include <sys/stat.h>
#include <unistd.h>
#include <fcntl.h>
#include <errno.h>
#include <stdlib.h>
#include <stdio.h>
#include <unistd.h>
#include <string.h>
#include <sys/ioctl.h>
#include <linux/perf_event.h>
#include <asm/unistd.h>
#include <cstring>
#include <vector>
#include <string>

#include "isomorphism.h"

const char* program_name;

using std::string;
using std::vector;

void set_up_graphs(int argc, char **argv, Graph &sub, Graph &graph);
vector<string> handle_args(int argc, char **argv);
void usage (FILE* stream, int exit_code);
Graph import_data(const char *filename);

static long perf_event_open(struct perf_event_attr *hw_event, pid_t pid,
    int cpu, int group_fd, unsigned long flags) {
```

```
  int ret;

  ret = syscall(__NR_perf_event_open, hw_event, pid, cpu,
      group_fd, flags);
  return ret;
}

int main(int argc, char **argv) {

  struct perf_event_attr pe;
  long long count;
  int fd;

  memset(&pe, 0, sizeof(struct perf_event_attr));
  pe.type = PERF_TYPE_HARDWARE;
  pe.size = sizeof(struct perf_event_attr);
  pe.config = PERF_COUNT_HW_CPU_CYCLES;
  pe.disabled = 1;
  pe.exclude_kernel = 1;
  pe.exclude_hv = 1;

  fd = perf_event_open(&pe, 0, -1, -1, 0);
  if (fd == -1) {
    fprintf(stderr, "Error opening leader %llx\n", pe.config);
    exit(EXIT_FAILURE);
  }

  Graph subgraph, graph;

  set_up_graphs(argc, argv, subgraph, graph);

  ioctl(fd, PERF_EVENT_IOC_RESET, 0);
  ioctl(fd, PERF_EVENT_IOC_ENABLE, 0);

  vector<int> isomorphism = find_isomorphism(subgraph, graph);

  ioctl(fd, PERF_EVENT_IOC_DISABLE, 0);
  read(fd, &count, sizeof(long long));

  if (isomorphism.size() == 0) {
    printf("No isomorphism found.\n");
  }

  else {
    printf("Isomorphism found! Assignments omitted, since we're just checking"
        " performance.\n");
  }

  printf("Searching for isomorphism took %lld CPU cycles\n", count);

  close(fd);
}

void set_up_graphs(int argc, char **argv, Graph &sub, Graph &graph) {

  program_name = argv[0];

  vector<string> args = handle_args(argc, argv);

  int interactive = atoi(args[0].c_str());

  char filename_default[] = "stdin";

  const char *graph_filename = (!interactive) ? args[2].c_str()
```

```
                                                          : filename_default;
  const char *sub_filename = (!interactive) ? args[3].c_str()
                                                          : filename_default;

  graph = import_data(graph_filename);

  sub = import_data(sub_filename);

  return;
}

vector<string> handle_args(int argc, char **argv) {
  // for getopt
  const char* const short_options = "hid";
  const struct option long_options[] = {
    { "help",  0, NULL, 'h' },
    { "interactive", 0, NULL, 'i'},
    { "debug", 0, NULL, 'd'},
    { NULL, 0, NULL, 0 }
  };

  vector<string> returnargs;
  returnargs.resize(4);
  int interactive = 0;
  int debug = 0;

  if (argc < 2) {
    usage(stderr, 1);
  }

  int next_option;
  do {
    next_option = getopt_long(argc, argv, short_options,
                              long_options, NULL);
    switch(next_option) {
      case 'h':
        usage(stdout, 0);
        // calling usage quits the program anyway but whatever
        // we'll put a break here anyway
        break;

      case 'i':
        interactive = 1;
        break;

      case 'd':
        debug = 1;
        break;

      case '?': // invalid option
        usage(stderr, 1);
        break;

      case -1: // no more options
        break;

      default: // something went very wrong if we got here
        abort();
    }
  }
  while (next_option != -1);

  // now that we've gone through all the options, OPIND points to first
  // nonoption argument. which is hopefully the first filename. unless
  // interactive was specified, in which case yell at the user.

  if (!interactive) {
    returnargs[2] = string(argv[optind]);
    returnargs[3] = string(argv[optind+1]);

  }

  if (debug) {
    fprintf(stderr,"Interactive set to %d. Debug is %d.\n", interactive, debug);
    if (!interactive) {
      fprintf(stderr,"Using file %s for graph and %s for subgraph.\n",argv[optind],argv[opt
    }
  }

  // put what we want to return in their places.
  returnargs[0] = std::to_string(interactive);
  returnargs[1] = std::to_string(debug);

  return returnargs;
}

void usage (FILE* stream, int exit_code) {
  fprintf(stream, "usage: %s [FILE] [OPTION]\n", program_name);
  fprintf(stream,
    "Options and arguments:\n"
    "FILE:                Space-separated file containing graph adjacency list. If edge weig
    "-h, --help:          Print this help message and exit.\n"
    "-i, --interactive:   Get space-separated graph adjacency list from stdin.\n"
    "-d, --debug:         Print debugging information.\n");

  exit(exit_code);
```

```
}

Graph import_data(const char *filename) {

  FILE *fd;
  if (strcmp(filename, "stdin") == 0) {
    fd = stdin;
  }

  else {
    fd = fopen(filename, "r");
    if (fd == NULL) {
      fprintf(stderr, "Could not open file %s for reading.\n", filename);
      perror("Error calling fopen()");
      exit(errno);
    }
  }

  char *line = NULL;
  size_t n = 0;

  Graph g;

  char *tempa, *tempb, *tempweight;
  char tempweight_default[] = "0";
  ssize_t bytes_read;
  // getline returns -1 on failure to read a line (including EOF)
  bytes_read = getline(&line, &n, fd);
  while (bytes_read != -1) {
    tempa = strtok(line, " ");
    // strtok returns NULL if the token (space in this case) was not found in the str
    // otherwise return the string up to the token (exclusive)
    if (tempa == NULL) {
      fprintf(stderr, "Error parsing file %s. Adjacency list must be of form 'node1 node2
          but line was %s\n", filename, line);
      exit(-1);
    }

    // if arg is null after a call to strtok, it'll keep reading after the position of the
    tempb = strtok(NULL, " ");
    if (tempb == NULL) {
      fprintf(stderr, "Error parsing file %s. Adjacency list must be of form 'node1 node2
          but line was %s\n", filename, line);
      exit(-1);
    }

    tempweight = strtok(NULL, " ");
    if (tempweight == NULL) {
      tempweight = tempweight_default;
    }

    int atempa = atoi(tempa);
    int atempb = atoi(tempb);
    int atempweight = atoi(tempweight);

    //printf("Edge is %d %d %d\n", atempa, atempb, atempweight);
    // this will also add the vertices if they don't exist
    // add_vertex is called from within add_edge if no vertex with the given value exists
    g.add_edge(atempa, atempb, atempweight);
    bytes_read = getline(&line, &n, fd);
  }

  if (fd != stdin) {
    int stat = fclose(fd);
    if (stat != 0) {
      perror("Error closing file");
      // we never wrote to the file so we probably don't even need to check for errors in t
      // but just kill the program if there's an error closing it
      exit(errno);
    }
  }

  // don't free line since it's null now

  return g;
}
```

Listing 12: Code used to check performance of C++ code

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