Algorithms and Computability

Finding maximum common subgraph

and minimum common supergraph

for given two graphs

Project description

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1   Introduction

The objective of this project is to try to solve two problems: finding a maximum common subgraph and finding a minimum common supergraph for any two given graphs. We assume that input graphs are directed, unweighted, don't have to be connected and don't have loops. In this document our team will describe both problems, propose an algorithm designed for each problem and explain how they work.

2   Problem description

There are a few common assumptions for both topics, hence they will be discussed before proceeding to the problems' descriptions. As it is mentioned in the introduction, we assume the input graphs to be:

- non-empty

- directed

- unweighted

- not necessarily connected

- without loops (i.e. without vertices connected to themselves)

- without multiple edges (we only allow a bidirectional connection between vertices, i.e. for any 2 vertices a, b in a graph, there can only be 1 edge from a to b, and one from b to a)

Moreover, all graphs processed by the algorithm will be represented using *adjacency matrices*, which store information about connections between vertices in an $|V| \times |V|$ arrays, where $|V|$ is the number of vertices in any given graph $G = (V, E)$. Considering described assumptions, all matrices in our program will contain only 0's or 1's, where a 1 at position (i, j) represents an edge directed from vertex i to vertex j. Naturally, for graphs without loops, all main diagonals entries of their matrices must be 0.

There are also terms, related to the adjacency matrices, that we will frequently use to describe algorithms in our documentation:

matrix permutation - a matrix representing a graph isomorphic to the original one, i.e. a matrix obtained by swapping corresponding rows and columns simultaneously (swapping rows 1 and 3 we must also swap columns 1 and 3)

isomorphism of graphs - an edge-preserving bijection between the vertex sets of two graphs

Adjacency Matrix

	0	1	2	3	4
0	0	1	1	0	0
1	0	0	1	0	1
2	0	0	0	1	0
3	0	0	0	0	1
4	0	0	0	0	0
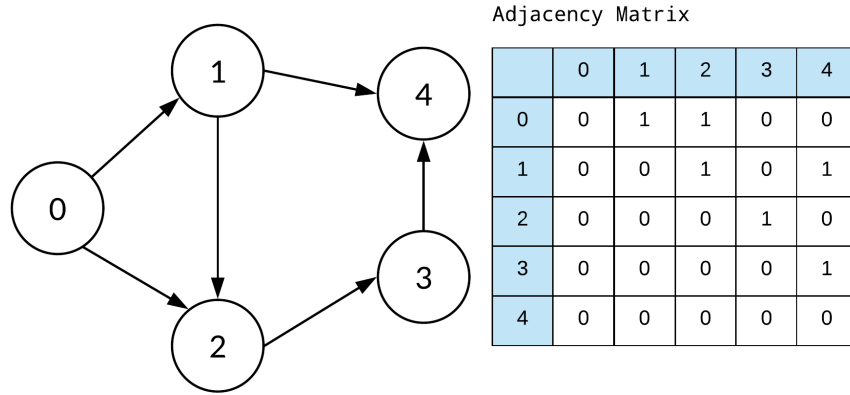
Example of a graph with its matrix representation

2.1 Maximum common subgraph

In graph theory, the *maximum common subgraph* may refer to either *maximum common induced subgraph*, which is an induced subgraph of two given graphs and has as many vertices as possible, or *maximum common edge subgraph*, which is a subgraph of two given graphs and has as many edges as possible. Given the choice, our team decided to implement an algorithm for finding the *maximum common edge subgraph* and the problem is defined as follows.

Given any 2 graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$, which satisfy the assumptions, the objective is to find a graph H isomorphic to both a subgraph of G_1 and a subgraph of G_2 with as many edges as possible. An isomorphism for graphs is an edge-preserving bijection between the vertex sets of G and H. This means that any two vertices u and v of G are adjacent in G if and only if the corresponding vertices in H are adjacent in H.
The search for maximum common subgraph is performed through a simple maximization of the sum of common edges counted for each matrix permutation of the larger of input graphs.

2.2 Minimum common supergraph

The *minimum common supergraph* of two graphs, G_1 and G_2, is defined as the smallest graph that includes, as subgraphs, both G_1 and G_2. We take into account any isomorphic representations of G_1 and G_2 as possible subgraphs of the desired minimum supergraph. Again, we aim to find the supergraph with the smallest number of edges possible and don't consider the vertices.

We observed that minimum common supergraph computation can be solved by means of maximum common subgraph computation, since both algorithms are based on counting edges of input graphs. The search for minimum common supergraph is performed by simple minimization of the sum of all edges found for each matrix permutation of the larger of input graphs.
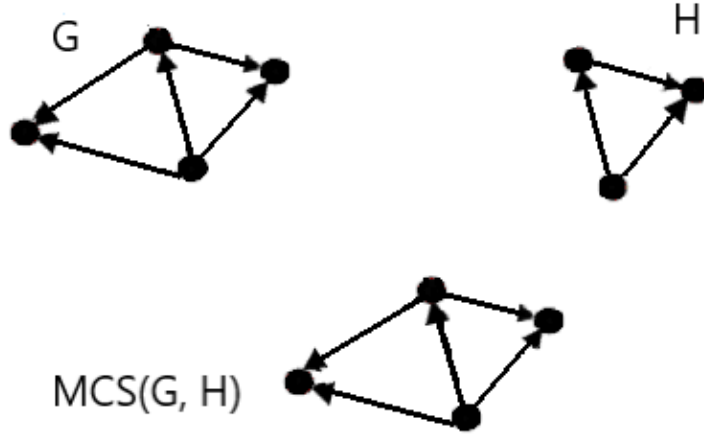
Minimum common supergraph

Finding maximal common subgraph and minimal common supergraph are NP-complete problems. In other words, they have a nondeterministic polynomial-time hardness and it is not known whether any polynomial-time algorithms will ever be found for solving those problems. Hence, our team designed an exact solution for each problem with factorial time complexity. The exact solutions are extremely inefficient and can be run only for very small graphs (i.e. with ≤ 10 vertices) to finish in reasonable amount of time. However, when an NP-complete problem must be solved, one approach is to use a polynomial algorithm to approximate the solution; the answer thus obtained will not necessarily be optimal but will be reasonably close. That is why, in order to run our algorithms for larger graphs, our team designed also an approximate solution with polynomial complexity for each problem, trying to make them as precise as possible.

3   Maximum common subgraph - Exact solution

The exact algorithm tries to obtain the solution by brute force, which means it enumerates all possible solutions and checks them against currently leading solution to return the best one. This approach is very straight-forward and it always chooses the best result but at the cost of very high time complexity (in this case - exponential complexity).

3.1 Pseudocode

Algorithm 1 *Maximum common subgraph (exact solution)*

1:   $M_1 \leftarrow$ Adjacency matrix representing graph G_1
2:   $M_2 \leftarrow$ Adjacency matrix representing graph G_2
3:   $V_1 \leftarrow$ Set of all vertices in graph G_1
4:   $V_2 \leftarrow$ Set of all vertices in graph G_2
Ensure: $|V_1| \geq |V_2| > 0$ $\triangleright$ Both matrices are not empty, and $M_1 \geq M_2$
5:   $maxSubGraph \leftarrow$ Empty Matrix
6:   $maxCommonEdges \leftarrow 0$
7:   **for each** $M = GetAllPermutations(M_1)$ **do**
8:      $V \leftarrow$ Set of all vertices in graph M
9:      $x \leftarrow 0$
10:     **while** $x \leq (|V_1| - |V_2|)$ **do**
11:        $y \leftarrow 0$
12:        **while** $y \leq (|V_1| - |V_2|)$ **do**
13:          $subMatrix \leftarrow GetSubMatrix(x, y, M, |V_2|)$
14:          $commonMatrix \leftarrow FindCommonMatrix(subMatrix, M_2)$
15:          $E \leftarrow$ Set of all edges in graph $commonMatrix$
16:          **if** $|E| > maxCommonEdges$ **then**
17:            $maxCommonEdges \leftarrow |E|$
18:            $maxSubGraph \leftarrow commonMatrix$
19:          **end if**
20:          $y \leftarrow y + 1$
21:        **end while**
22:        $x \leftarrow x + 1$
23:     **end while**
24: **end for**
25: **return** $maxSubGraph$

This solution works by firstly obtaining all possible permutations of the larger matrix with *GetAllPermutations* function. Then it iterates through all of the obtained matrices and compares each permutation of the larger matrix with the smaller matrix in the following way: from larger matrix take all possible submatrices of the same size as the smaller matrix (each one returned by method *GetSubMatrix*) and obtain an "intersection" of those two matrices with method *FindCommonMatrix*. This method returns a matrix with 1's only in entries where both input matrices have 1's as well and all other entries are 0. Then, the algorithm counts edges in the obtained "intersection" matrix and if the value is highest so far, the results are saved by overwriting the *maxCommonEdges* and *maxSubGraph* variables. After the algorithm finishes, the best solution saved in the *maxSubGraph* variable is returned.

NOTE: All methods used in this algorithm are common for presented solutions and are described in section 7.

3.2 Complexity analysis

For the exact solution, the upper bound of complexity will be analysed. As per the definition, $g(n)$ is an upper bound of $f(n)$ (denoted by $f = \mathcal{O}(g)$) if the following condition holds:

$$f = \mathcal{O}(g)) \iff \exists_{c>0} \exists_{n_0 \in N} \forall_{n>n_0} c * g(n) \geq f(n)$$

Firstly, we assume that the input matrices M_1 and M_2 have the respective numbers of vertices $|V_1| = n$ and $|V_2| = k$ and $n \geq k$, hence we can use only n to bound the time complexity. The algorithm starts by generating all possible permutations of the larger matrix which gives the complexity of $\mathcal{O}(n!)$. Then, iterating through all those permutations adds another $\mathcal{O}(n!)$ which needs to be multiplied by $\mathcal{O}(n^2)$ because of the nested loop. Then, for current permutation of the larger matrix we perform two operations: *GetSubMatrix* ($\mathcal{O}(n^2)$ complexity) and *FindCommonMatrix* (also $\mathcal{O}(n^2)$). The final time complexity of the whole algorithm can be denoted as function T:

$$T(n) = n! + n! \cdot n \cdot n \cdot (n^2 + n^2)$$

$$T(n) = n! \cdot n^2 \cdot n^2$$

$$T(n) = \mathcal{O}(n! \cdot n^4)$$

As we can see, the complexity of this algorithm is extremely high and adding even one vertex to any of the input matrices would increase the computation time exponentially. However, at a cost of this tremendously high complexity, we can be sure that the algorithm finds the best possible solution and the resulting graph is indeed the maximum common subgraph of the input graphs.

4 Minimum common supergraph - Exact solution

The exact algorithm for the minimum common supergraph problem is very similar to the previous one - it also enumerates all possible solutions and checks them against each other to return the most optimal one. However, the similarity also applies for the exponential complexity, which makes this solution extremely inefficient.

4.1 Pseudocode

Algorithm 2 *Minimum common supergraph (exact solution)*

1: $M_1 \leftarrow$ Adjacency matrix representing a graph G_1
2: $M_2 \leftarrow$ Adjacency matrix representing a graph G_2
3: $V_1 \leftarrow$ Set of all vertices in a graph G_1
4: $V_2 \leftarrow$ Set of all vertices in a graph G_2
Ensure: $|V_2| \geq |V_1| > 0$ ▷ Both matrices are not empty and $M_2 \geq M_1$
5:    $SmallestSuperGraph \leftarrow$ Empty Matrix
6:    $minCommonEdges \leftarrow$ Maximal integer number
7: **for each** $M = GetAllIsomporphicGraphsTo(M_2)$ **do**
8:      $x \leftarrow 0$
9:      **while** $x \leq (|V_2| - |V_1|)$ **do**
10:        $y \leftarrow 0$
11:        **while** $y \leq (|V_2| - |V_1|)$ **do**
12:          $newMatrix \leftarrow$ Copy of M
13:          $newMatrix \leftarrow InsertEdgesToMatrixAt(newMatrix, x, y, M_1)$
14:          **if** $|newMatrix.Edges| < minCommonEdges$ **then**
15:            $minCommonEdges \leftarrow newMatrix.Edges$
16:            $SmallestSuperGraph \leftarrow newMatrix$
17:          **end if**
18:          $y \leftarrow y + 1$
19:        **end while**
20:        $x \leftarrow x + 1$
21:      **end while**
22: **end for**
23: **return** $SmallestSuperGraph$

This algorithm checks all possible common supergraphs and saves the smallest one. It starts by generating all graphs isomorphic to the larger graph (i.e. one with more vertices). For every found matrix permutation, denoted by variable M, we "fit" the smaller matrix M_1 into the larger matrix permutation M in the following way: left upper corner of M_1 is placed in the current (x, y) position of the larger matrix M and all edges that are present in the smaller matrix are copied into corresponding places in M. This is done by the method *InsertEdgesToMatrixAt* which returns a new matrix with edges from both input matrices. The number of edges in this resulting matrix, denoted by the variable *newMatrix*, is then compared with the lowest saved value so far and if its even lower, the best solution stored in the *SmallestSuperGraph* variable is overwritten. After the algorithm finishes, the *SmallestSuperGraph* is returned as the most optimal solution found.

Generally, using the variables defined in the algorithm, the search for the mimnimum common supergraph is based on the following assumptions:

If every found position in M is described by x and y then the common supergraph of M and B is a graph C defined as follows:

$$M = \{a_{0,0}, a_{0,1}, ..., a_{n,n}\}$$

$$B = \{b_{0,0}, b_{0,1}, ..., b_{m,m}\}$$

$$C = \{c_{0,0}, c_{0,1}, ..., c_{n,n}\}$$

$$a_{i,j} = 1 \Rightarrow c_{i,j} = 1$$

$$b_{i,j} = 1 \Rightarrow c_{i-x,j-y} = 1$$

Such a definition of C represents a common supergraph for every isomorphic matrix M and every correct position (x, y) in M. Minimal common supergraph is a graph C that has the smallest number of edges.

4.2 Complexity analysis

Similarly to the maximum common subgraph algorithm, we firstly assume that the input matrices M_1 and M_2 have the respective numbers of vertices $|V_1| = k$ and $|V_2| = n$ and $n \geq k$. Again, for the simplicity of the notation we define the time complexity as a function of n, as the size of greater matrix bounds the worst possible scenario of the solution. This algorithm also starts by generating all possible permutations of the larger matrix and iterating through them ($\mathcal{O}(n!)$ complexity). For each permutation, it then performs a doubly nested loop with complexity $\mathcal{O}(n^2)$ in which there is only one more complex method - *InsertEdgesToMatrixAt* with complexity $\mathcal{O}(n^2)$. Hence, the complexity of the whole algorithm can be represented by:

$$T(n) = n! + n! \cdot n^2 \cdot n^2$$

$$T(n) = n! \cdot n^2 \cdot n^2$$

$$T(n) = \mathcal{O}(n! \cdot n^4)$$

Complexity of this algorithm is the same as that of the maximum common subgraph solution. And again, at the cost of extreme inefficiency we obtain the best possible solution to the minimum common supergraph problem.

5 Maximum common subgraph - Approximate solution

Quite opposite to the brute force approach, in approximate solution the goal is not to find the best possible answer, but to find one closest to the optimal, with as low time complexity as possible. In this case, we aim to reduce the complexity to a polynomial time in order to be able to test the solution for graphs larger than just 10 vertices.

This algorithm is very similar to the exact solution - to approximate the possible maximum common subgraph we decided to "sort" input graphs instead of obtaining all permutations of larger graph. "Sorting" transforms the input graphs into similar forms and hence, increases the probability of finding the best solution. This way we should end up with a maximum common subgraph close to the one obtained by the exact algorithm.

5.1 Pseudocode

Algorithm 3 *Maximum common subgraph (approximate solution)*

1: $M_1 \leftarrow$ Adjacency matrix representing graph G_1
2: $M_2 \leftarrow$ Adjacency matrix representing graph G_2
3: $V_1 \leftarrow$ Set of all vertices in graph G_1
4: $V_2 \leftarrow$ Set of all vertices in graph G_2
Ensure: $|V_1| \geq |V_2| > 0$ ▷ Both matrices are not empty and $M_1 \geq M_2$
5: $SortedMatrixA \leftarrow TransformToSortedForm(M_1)$
6: $SortedMatrixB \leftarrow TransformToSortedForm(M_2)$
7: $maxSubGraph \leftarrow$ Empty Matrix
8: $maxCommonEdges \leftarrow 0$
9: $x \leftarrow 0$
10: **while** $x \leq |V_1| - |V_2|$ **do**
11:      $y \leftarrow 0$
12:      **while** $y \leq |V_1| - |V_2|$ **do**
13:          $subMatrix \leftarrow GetSubMatrix(x, y, M_1, |V_2|)$
14:          $commonMatrix \leftarrow FindCommonMatrix(subMatrix, M_2)$
15:          $E \leftarrow$ Set of all edges in graph $commonMatrix$
16:          **if** $|E| > maxCommonEdges$ **then**
17:             $maxCommonEdges \leftarrow |E|$
18:             $maxSubGraph \leftarrow commonMatrix$
19:          **end if**
20:          $y \leftarrow y + 1$
21:      **end while**
22:      $x \leftarrow x + 1$
23: **end while**
24: **return** $maxSubGraph$

In this algorithm, instead of generating isomorphic graphs, the input graphs are firstly transformed into "sorted" forms, i.e. they have as many 1's as possible in the upper left part of the matrix. It is done by the method *TransformToSortedForm* which is described in more detail in section 7. Then, just as in the exact solution, the algorithm checks each part of the larger matrix (M_1) of size equal to the smaller input matrix size ($|V_2|$) against the smaller matrix (M_2), finds an "intersection" matrix between those two and counts its edges. The obtained number of edges is then compared with the highest value so far. If it is even higher, the results are saved by overwriting the *maxCommonEdges* and *maxSubGraph* variables, which, after the algorithms finishes, hold the best approximated solution to the problem.

5.2 Complexity analysis

We assume that the input matrices M_1 and M_2 have the respective numbers of vertices $|V_1| = n$ and $|V_2| = k$ and $n \geq k$. Again, we can bound the complexity by the size of greater matrix - n. This algorithm firstly sorts the two input matrices and this operation has time complexity $\mathcal{O}(n^2 + n^2)$ as described in section 7. Then, iterating through nested loop of size n gives $\mathcal{O}(n^2)$ complexity which has to be multiplied by $\mathcal{O}(n^2) + \mathcal{O}(n^2)$ from *GetSubMatrix* and *FindCommonMatrix* functions. In overall, the time complexity of the whole algorithm can be denoted as function T:

$$T(n) = n^2 + n^2 + n \cdot (n \cdot (n^2 + n^2))$$

$$T(n) = n^2 + n^2 \cdot n^2$$

$$T(n) = \mathcal{O}(n^4)$$

We obtained a polynomial time complexity which is much better than in the exact solution and would allow for testing the algorithm against much bigger inputs.

6 Minimum common supergraph - Approximate solution

The approximate solution for minimum common supergraph aims at reducing the complexity to a polynomial time. This algorithm is also very similar to its exact counterpart and instead of generating all permutations of larger matrix, it transforms input matrices into "sorted" forms with *TransformToSortedForm* function. Then, the main loop goes through the larger matrix in such a way that at each iteration of the loop, variables x and y describe the start position in the larger matrix at which the upper left corner of the smaller matrix should be "fitted". Then, the larger matrix is copied and all edges from the smaller matrix are inserted into the copied matrix at appropriate positions (x, y) - this logic is the same as in the exact solution. Finally, the graph with inserted edges is compared with the best result so far and saved if it has even less edges than the current result. At the end, the algorithm returns the approximated minumum common supergraph which should be close to the optimal solution.

6.1 Pseudocode

Algorithm 4 *Minimum common supergraph (approximate solution)*

1: $M_1 \leftarrow$ Adjacency matrix representing a graph G_1
2: $M_2 \leftarrow$ Adjacency matrix representing a graph G_2
3: $V_1 \leftarrow$ Set of all vertices in a graph G_1
4: $V_2 \leftarrow$ Set of all vertices in a graph G_2
Ensure: $|V_2| \geq |V_1| > 0$ ▷ Both matrices are not empty and $M_2 \geq M_1$
5: $M_1 \leftarrow TransformToSortedForm(M_1)$
6: $M_2 \leftarrow TransformToSortedForm(M_2)$
7: $SmallestSuperGraph \leftarrow$ Empty Matrix
8: $minCommonEdges \leftarrow$ Maximal integer number
9: $x \leftarrow 0$
10: **while** $x \leq (|V_2| - |V_1|)$ **do**
11:      $y \leftarrow 0$
12:      **while** $y \leq (|V_2| - |V_1|)$ **do**
13:          $newMatrix \leftarrow$ Copy of M
14:          $newMatrix \leftarrow InsertEdgesToMatrixAt(newMatrix, x, y, B)$
15:          **if** $|newMatrix.Edges| < minCommonEdges$ **then**
16:              $minCommonEdges \leftarrow newMatrix.Edges$
17:              $SmallestSuperGraph \leftarrow newMatrix$
18:          **end if**
19:          $y \leftarrow y + 1$
20:      **end while**
21:      $x \leftarrow x + 1$
22: **end while**
23: **return** $SmallestSuperGraph$

6.2 Complexity analysis

Just as in all previous cases, we firstly need to assume that the input matrices M_1 and M_2 have the respective numbers of vertices $|V_1| = k$, $|V_2| = n$ and $n \geq k$. The algorithm starts by sorting both input matrices which is done in $n^2 + n^2$ time, as described in the *TransformToSortedForm* function. Then, iterating through part of the larger matrix has $(\mathcal{O}(n^2)$ complexity. In each loop iteration, there are only two costly operations - copying matrix and inserting edges into larger matrix, which is done in n^2 and n^2 time. Since $n \geq k$, we can use only n to denote the worst-case scenario of the algorithm and the complexity can be represented by:

$$T(n) = n^2 + n^2 + n \cdot n \cdot (n^2 + n^2)$$

$$T(n) = n^2 + \cdot n^2 \cdot n^2$$

$$T(n) = \mathcal{O}(n^4)$$

This algorithm has polynomial time complexity which is incomparably better than in the brute force approach. We are able to obtain reasonably optimal solutions in a fraction of the exact algorithm time.

7 Common methods

This section describes methods used in all previously discussed solutions. Each method is presented with a pseudocode, a description of how it works and its time complexity analysis.

1) **GetSubMatrix**

Algorithm 5

1: **procedure** GetSubMatrix($xIndex, yIndex, Matrix, size$)
2:     $SubMatrix \leftarrow$ Empty Matrix
3:     $i \leftarrow$ xIndex
4:     **while** $i < xIndex + size$ **do**
5:         $j \leftarrow yIndex$
6:         **while** $j < yIndex + size$ **do**
7:             SubMatrix[i - xIndex][j - yIndex] = Matrix[i][j]
8:             $j \leftarrow j + 1$
9:         **end while**
10:         $i \leftarrow i + 1$
11:     **end while**
12:     **return** $SubMatrix$
13: **end procedure**

The *GetSubMatrix* method returns a square submatrix of given size which starts at position $(xIndex, yIndex)$ in the input matrix. To obtain the result, it copies numbers from the input matrix row by row, starting from the row given by $xIndex$; in each row it starts from the column given by $yIndex$ and proceeds to the next row when $size$ numbers are copied.

Time complexity of this function is $T(n) = n \cdot n = \mathcal{O}(n^2)$, where $n = size$ of submatrix it returns. It is a very simple method iterating through a 2-dimensional array and copying appropriate values and hence it has quadratic complexity.

2) FindCommonMatrix

Algorithm 7

1: **procedure** FindCommonMatrix(M_1, M_2)
2:     $V_1 \leftarrow$ Set of all vertices in graph M_1
3:     $V_2 \leftarrow$ Set of all vertices in graph M_2
Ensure: $|V_1| == |V_2|$ ▷ Both matrices have the same size
4:     $CommonMatrix \leftarrow$ Copy of M_1
5:     $i \leftarrow 0$
6:     **while** $i < |V_1|$ **do**
7:         $j \leftarrow 0$
8:         **while** $j < |V_1|$ **do**
9:             **if** $M_1[i][j] == 1$ and $M_2[i][j] == 0$ **then**
10:                 CommonMatrix[i][j] = 0
11:             **end if**
12:             $j \leftarrow$ j + 1
13:         **end while**
14:         $i \leftarrow$ i + 1
15:     **end while**
16:     **return** CommonMatrix
17: **end procedure**

The procedure *FindCommonMatrix* is applicable only for two matrices of the same size. It returns a third matrix of the same size which has only those edges which are present in both input matrices. To obtain the resulting matrix, it copies the first given matrix, iterates through both input matrices and checks each entry. We have four cases:

- If the entry is equal to 1 in both matrices, then it is a common edge. It is already marked as 1 in the resulting matrix, so no action needs to be taken.

- If the entry equals 1 in the first matrix and 0 in the second one, then it is not a common edge. This entry needs to be marked as 0 in the resulting matrix.

- If the entry is equal to 0 in the first matrix and to 1 in the second one, then it is also not a common edge. However, it is already marked as 0 in the resulting matrix, so no action needs to be taken.

- If the entry is equal to 0 in both matrices, then it is not a common edge and again, it is already marked as 0 in the resulting matrix.

Hence, the algorithm only needs to check for the second case, apply necessary changes and after iterating through the whole resulting matrix - return it.

Time complexity of this function is again $T(n) = n \cdot n = \mathcal{O}(n^2)$, where n is the size of either of the input matrices. Just as in the previous case, iterating through a 2-dimensional array gives quadratic complexity.

3) **GetAllIsomporphicGraphsTo(Matrix)**

Algorithm 8

1: **procedure** GetAllIsomporphicGraphsTo($Matrix$)
2:     $Matrix \leftarrow$ Matrix that will be transformed
3:     $P \leftarrow$ All permutations without repetitions of numbers from 0 to $|V_{Matrix}| - 1$
4:     $Result \leftarrow$ Empty array
5:     **for each** $array \leftarrow P$ **do**
6:         $newM \leftarrow$ Copy $Matrix$
7:         $i \leftarrow 0$
8:         **while** $i \leq array.size$ **do**
9:             **if** $array[i] \neq i$ **then**
10:                 $newM \leftarrow SwapColumn(newM, array[i], i)$
11:                 $newM \leftarrow SwapRow(newM, array[i], i)$
12:                 $array \leftarrow Swap(array, array[i], i)$
13:             **end if**
14:             $i \leftarrow i + 1$
15:         **end while**
16:         $Result.append(newM)$
17:     **end for**
18:     **return** $Result$
19: **end procedure**

This function returns all graphs that are isomorphic to the given graph. It firstly generates all permutations of sequences of numbers from 0 to $|V_{Matrix}| - 1$. Each sequence represents the order of vertices in adjacency matrix of a graph. Then, the method iterates through the current sequence permutation and swaps appropriate rows and columns of the input matrix, to match the order of numbers in the permutation sequence. The resulting matrix is added to the list of all generated isomorphic graphs, which is then returned as a final result.

Time complexity of this function is $T(n) = n! + n! \cdot n = \mathcal{O}(n! \cdot n)$, where n is the number of vertices of the input graph. Because there are $n!$ permutations without repetitions of a set with size n and for every permutation the algorithm performs a loop with complexity $\mathcal{O}(n)$, the complexity of this function is very high and reaches $\mathcal{O}(n! \cdot n)$.

4) **TransformToSortedForm**

Algorithm 9

1: **procedure** TransformToSortedForm($Matrix$)
2:     $i \leftarrow 0$
3:     **while** $i \le |Matrix.Vertices|$ **do**
4:         $j \leftarrow 0$
5:         **while** $j \le |Matrix.Vertices|$ **do**
6:             **if** $DegRow(i) + DegCol(i) > DegRow(j) + DegCol(j)$ **then**
7:                 $newM \leftarrow SwapColumn(Matrix, i, j)$
8:                 $newM \leftarrow SwapRow(Matrix, i, j)$
9:             **end if**
10:             $j \leftarrow j + 1$
11:         **end while**
12:         $i \leftarrow i + 1$
13:     **end while**
14:     **return** $Matrix$
15: **end procedure**

This function creates an adjacency matrix of the graph isomorphic to the given graph. The obtained matrix has rows and columns sorted in such a way that most of the ones are placed in the left top corner and most of the zeros are placed in the right bottom corner.

The algorithm structure is very similar to a simple bubble sort. Every index is compared with every other index in the matrix and if they are in the wrong order they are swapped. The value of the index is defined by the following function: $DegRow(i) + DegCol(i)$. This means that the value of given index i is defined as the number of edges (sum of 1's) in i-th column and i-th row. If there exists i and j such that the value of index j is less than the value of index i, then row i is swapped with row j, and column i is swapped with column j. After checking all combinations of i and j we can be sure that the given matrix is transformed to most optimal, sorted form.

```
0 1 1 0 0 1 0 1 1 1 1          0 1 1 1 1 1 1 0 0 1 0
0 0 1 0 1 0 1 0 1 0 0          1 0 1 0 1 0 1 1 1 1 0 1
0 0 0 1 0 0 0 0 1 1 0          1 0 0 0 1 0 1 0 1 1 0
0 0 0 0 0 0 1 0 1 0 1          1 1 1 0 1 1 1 1 0 1 1
1 0 0 0 0 0 0 0 0 0 0          0 1 1 0 0 0 0 0 1 0 0
1 0 1 0 1 0 1 0 0 1 0          1 0 1 0 1 0 0 1 0 0 1
1 0 0 1 0 0 0 0 0 0 0          0 1 0 0 1 0 0 1 0 0 1
1 0 0 0 0 1 0 0 0 1 0          1 0 0 0 0 0 0 0 1 0 0
1 1 1 1 1 0 1 0 0 1 0          0 1 0 1 0 0 0 1 0 0 0
1 1 1 1 0 0 0 1 0 0 0          1 0 1 0 0 1 0 0 0 0 0
1 1 1 0 1 1 1 1 1 1 0          1 0 0 0 0 0 0 0 0 0 0
```

| Example matrix before translation | Example matrix after translation |

It is not possible to accurately place all 1's closest to one of matrix corners because the
represented graph will stop being isomorphic to the original one. But generally, rows
with the most 1's are placed at the top, and columns with the most 1's are placed on
the left of the matrix, hence this algorithm aims to make the adjacency matrices of two
input graphs as similar to each other as possible. Thanks to that, algorithms which use
matrix permutations can be approximated with higher accuracy, without the need to
generate all possible solutions.

Time complexity of this function is $T(n) = n \cdot n = \mathcal{O}(n^2)$, since we have only one nested
loop and thanks to graphs being represented with adjacency matrices, the operations
of swapping rows and columns have constant complexity.

5) **InsertEdgesToMatrix**

This function is used in the minimum common supergraph problem. It iterates through
a submatrix of size $|V_{M_S}|$ x $|V_{M_S}|$ from the larger input matrix M_B, starting from the
given position (x, y). If at a given position there is an edge in the smaller matrix, it is
inserted into the larger matrix at a corresponding position. After the algorithm finishes,
the larger matrix stores all edges from both graphs and makes a single solution for the
minimum common subgraph problem.

Algorithm 10

1: **procedure** InsertEdgesToMatrixAt(M_B, x, y, M_S)

Ensure: $|M_B| \geq |M_S| > 0$ ▷ M_B is the bigger matrix

2:     $i \leftarrow x$

3:     **while** $i \leq |V_{M_B}|$ and $i - x \leq |V_{M_S}|$ **do**

4:        $j \leftarrow y$

5:        **while** $j \leq |V_{M_B}|$ and $j - y \leq |V_{M_S}|$ **do**

6:           **if** $M_S[i - x][j - y] == 1$ **then**

7:             $M_B[i][j] = M_S[i - x][j - y]$

8:           **end if**

9:           $j \leftarrow j + 1$

10:        **end while**

11:        $i \leftarrow i + 1$

12:     **end while**

13: **end procedure**

Time complexity of this function is $T(n) = n \cdot n = \mathcal{O}(n^2)$, where n is the number of vertices in the smaller graph. The complexity is again quadratic thanks to one nested loop with simple comparisons and assignment operations.

8   Results

The algorithms were tested on randomly generated pairs of matrices, which were divided into two sets based on the size of the larger matrix.

To test the speed of the exact algorithms we used matrices of sizes from 4 up to 10 vertices with 3 pairs of matrices for each size. For testing the approximate algorithms we used graphs with sizes from 10 up to 95, incremented by 5 (i.e. 10, 15, ..., 90, 95) and for each size 50 pairs of matrices were generated. For every set of matrices with the same number of vertices in the larger graph, we calculate the average value of the results of the given algorithm to have a better representation of how the algorithm behaves for graphs of a given size.

To test the difference in accuracy between exact and approximate algorithms we used matrices with sizes from 4 up to 10 vertices (3 pairs of matrices for each size). Similarly, to test the difference in accuracy between approximate algorithms with and without sorting the input matrices, we used from 10 up to 95, incremented by 5 (i.e. 10, 15, ..., 90, 95), with 3 pairs of matrices generated for each size.

We decided to check our results in the following four categories.

8.1 Speed tests of approximate algorithms
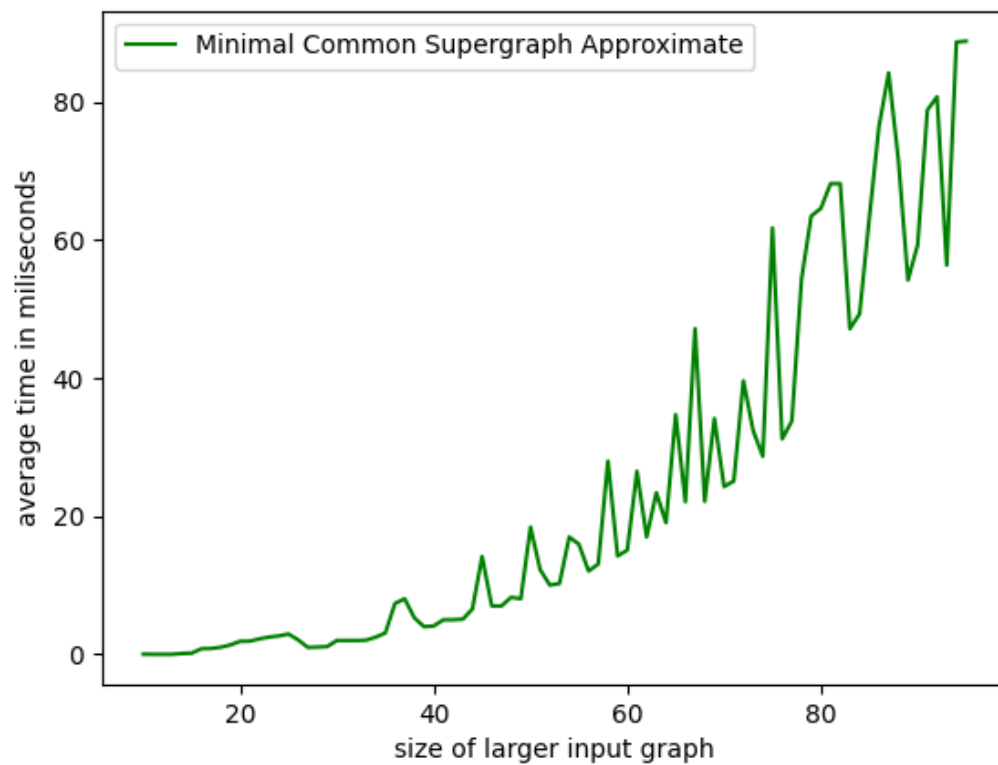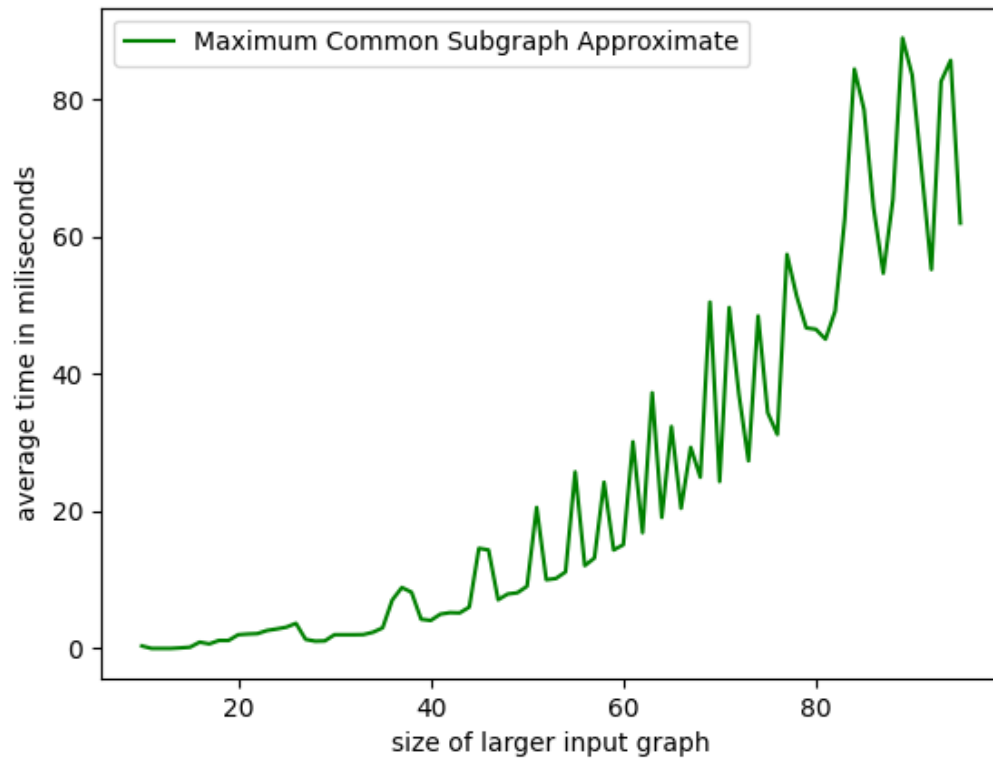
We can see that approximate algorithms are very fast as it takes around 0.1 seconds to find a maximal common subgraph for graphs with around 80 vertices. Both algorithms (for maximal subgraph and minimal supergraph) have similar time execution because they have the same complexity. We can see some distortions which will appear even for tests on high amount of graphs, because the y scale is very precise, and even a small change of a couple of milliseconds results in big distortion. The most important thing we can take from the graphs is that time of algorithms roughly follows the quadratic complexity.

Comparison of the time execution of the maximal common subgraph and minimal common supergraph algorithms looks as follows:
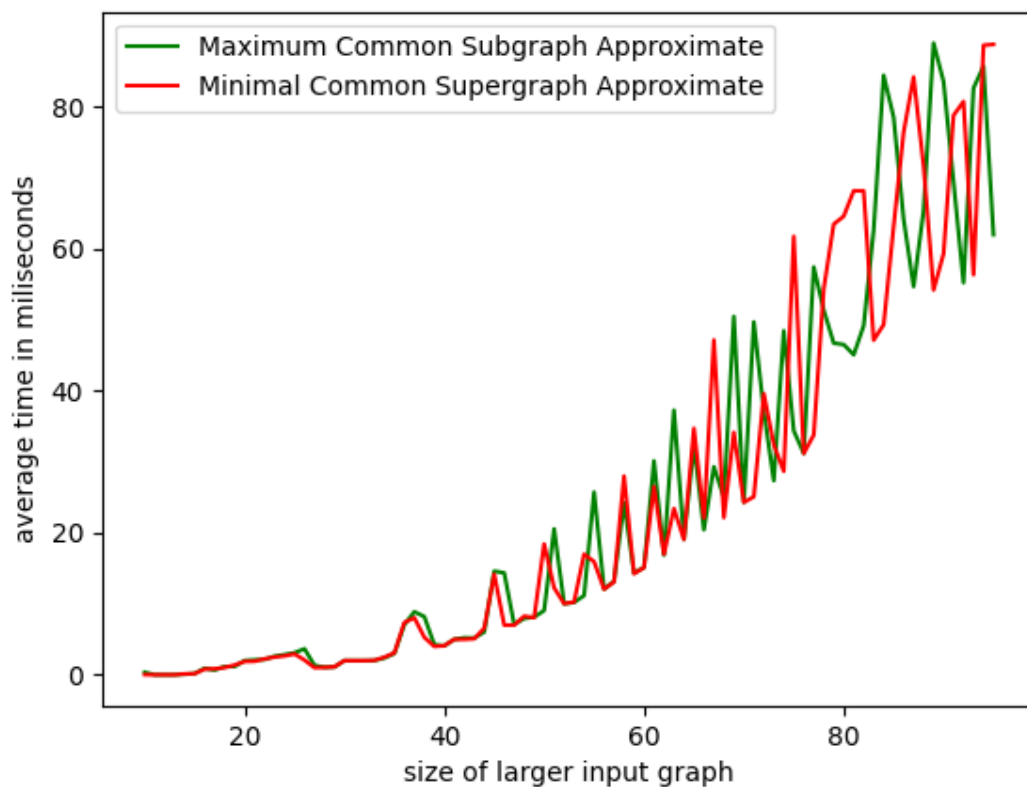
As we can see, time execution for both algorithms is very similar. It comes from the fact that both algorithms were run on the same set of graphs and have the same complexity.

8.2   Speed tests of exact algorithms
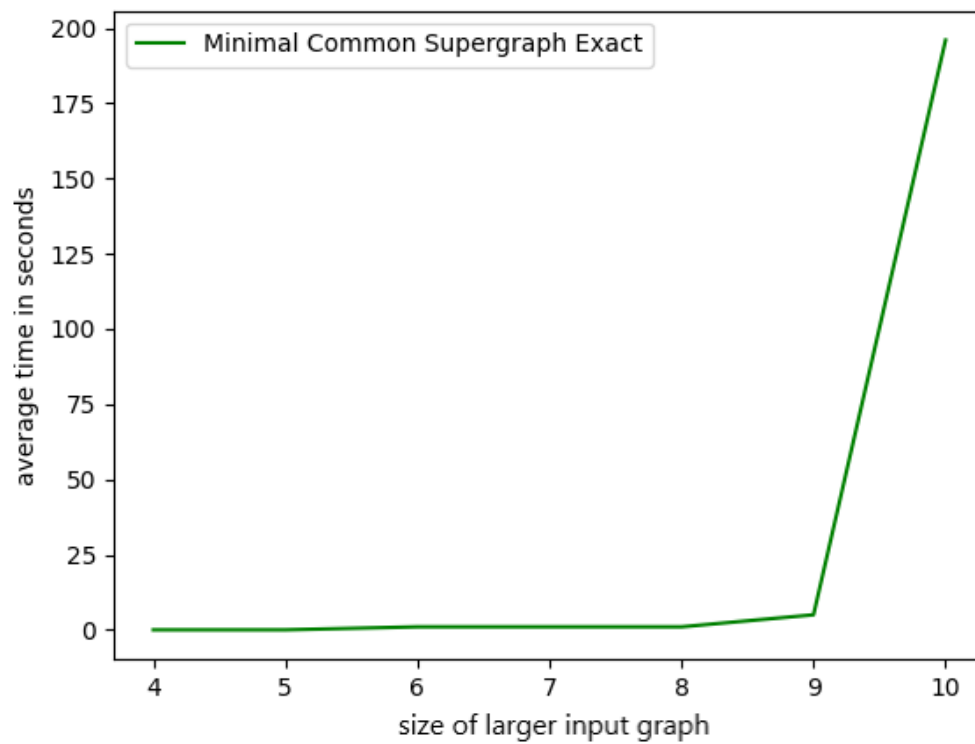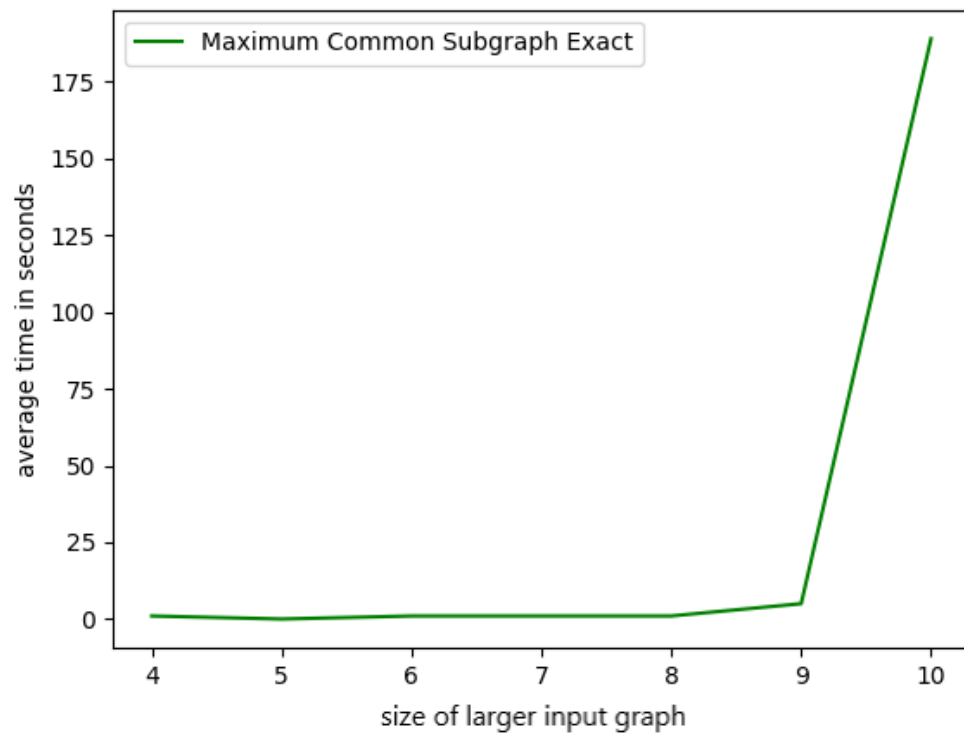
Again, we can see that execution times of the exact algorithms are very similar. This is the result we expected, because the time complexity of both algorithms is almost the same and the plots clearly illustrate the exponential growth of their performance. The time of execution reaches around 3 minutes for graphs with only 10 vertices, so we can easily deduce it would be impossible to run those algorithms for larger graphs on a regular computer.

8.3 Comparison of approximate and exact algorithms
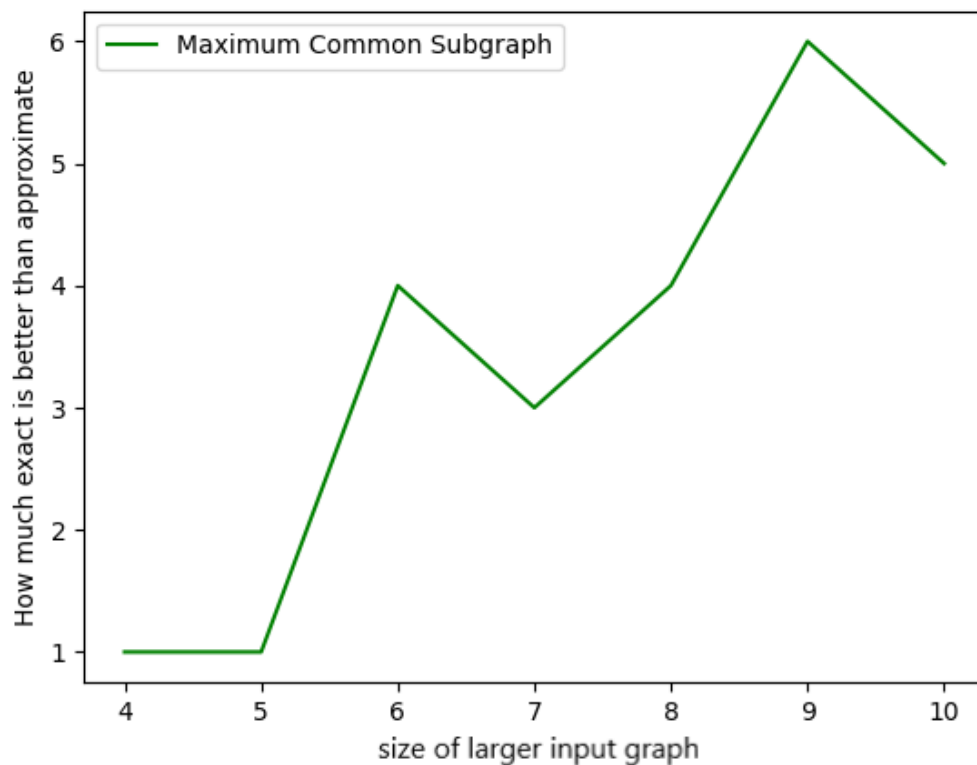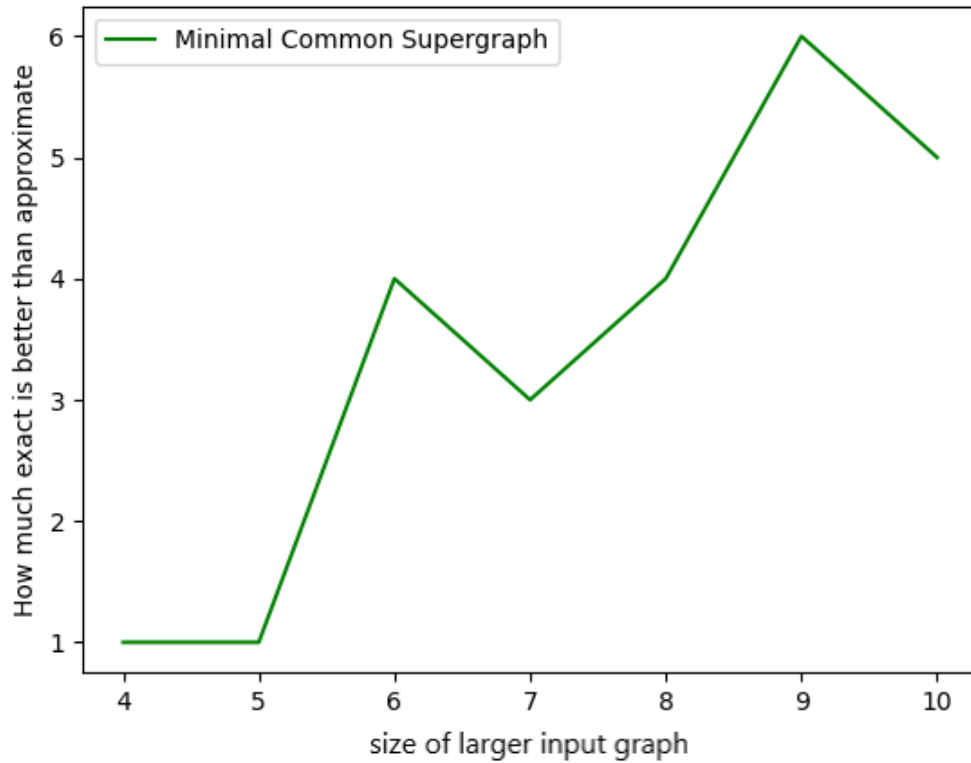
The above diagrams present the difference between number of edges of the graph resulting from the approximate algorithm and the number of edges resulting from the exact algorithm. We can easily see that as the size of input graphs increases, the accuracy approximate algorithm is getting worse. But the most interesting fact is that those two diagrams are identical. We checked both algorithms on many examples and after taking any two random graphs, the difference between the number of edges found by exact algorithm and approximate algorithm for the maximal common subgraph problem was always the same as the difference between number of edges for exact and approximate solutions for minimal common supergraph. Below we present one of the examples from the console output:

```
G1 sorted
(4 5 3 7 6 2 1)
----------------------
0 1 1 1 1 1 0
1 0 0 0 1 0 1
1 1 0 0 0 1 0
1 0 1 0 1 0 0
0 0 0 1 0 0 0
1 0 0 0 0 0 0
0 1 0 0 0 0 0

Max Common Subgraph (Approximate)
EDGES: 5
0 0 0 1 0 1 0
1 0 0 0 1 0 0
1 0 0 0 0 0 0
0 0 0 0 0 0 0
0 0 0 0 0 0 0
0 0 0 0 0 0 0
0 0 0 0 0 0 0
```

```
G2 sorted
(1 3 2 6 4 7 5)
----------------------
0 0 0 1 0 1 0
1 0 0 1 1 0 0
1 0 0 0 0 0 0
0 1 0 0 0 0 0
0 0 1 0 0 0 0
0 0 1 0 0 0 0
0 0 0 0 0 0 0
```

```
G1 permuted
(4 5 7 1 2 6 3)
----------------------
0 1 1 0 1 1 1
1 0 0 1 0 1 0
1 0 0 0 0 1 1
0 1 0 0 0 0 0
1 0 0 0 0 0 0
0 0 1 0 0 0 0
1 1 0 0 1 0 0

Max Common Subgraph (Exact)
EDGES: 8
0 0 0 0 0 1 1
1 0 0 0 0 0 0
1 0 0 0 0 1 0
0 1 0 0 0 0 0
0 0 0 0 0 0 0
0 0 1 0 0 0 0
0 1 0 0 0 0 0
```

```
G2 original
(1 2 3 4 5 6 7)
----------------------
0 0 0 0 0 1 1
1 0 0 0 0 0 0
1 0 0 1 0 1 0
0 1 0 0 0 0 0
0 0 0 0 0 0 0
0 0 1 0 0 0 0
0 1 0 0 0 0 0
```

```
 G1 sorted                          G2 sorted
(4 5 3 7 6 2 1)                    (1 3 2 6 4 7 5)
---------------------              ---------------------
 0  1  1  1  1  1  0                0  0  0  1  0  1  0
 1  0  0  0  1  0  1                1  0  0  1  1  0  0
 1  1  0  0  0  1  0                1  0  0  0  0  0  0
 1  0  1  0  1  0  0                0  1  0  0  0  0  0
 0  0  0  1  0  0  0                0  0  1  0  0  0  0
 1  0  0  0  0  0  0                0  0  1  0  0  0  0
 0  1  0  0  0  0  0                0  0  0  0  0  0  0

 Min Common Supergraph (Approximate)
 EDGES: 21
 0  1  1  1  1  1  0
 1  0  0  1  1  0  1
 1  1  0  0  0  1  0
 1  1  1  0  1  0  0
 0  0  1  1  0  0  0
 1  0  1  0  0  0  0
 0  1  0  0  0  0  0
```

```
 G1 permuted                        G2 original
(4 5 7 1 2 6 3)                    (1 2 3 4 5 6 7)
---------------------              ---------------------
 0  1  1  0  1  1  1                0  0  0  0  0  1  1
 1  0  0  1  0  1  0                1  0  0  0  0  0  0
 1  0  0  0  0  1  1                1  0  0  1  0  1  0
 0  1  0  0  0  0  0                0  1  0  0  0  0  0
 1  0  0  0  0  0  0                0  0  0  0  0  0  0
 0  0  1  0  0  0  0                0  0  1  0  0  0  0
 1  1  0  0  1  0  0                0  1  0  0  0  0  0

 Min Common Supergraph (Exact)
 EDGES: 18
 0  1  1  0  1  1  1
 1  0  0  1  0  1  0
 1  0  0  1  0  1  1
 0  1  0  0  0  0  0
 1  0  0  0  0  0  0
 0  0  1  0  0  0  0
 1  1  0  0  1  0  0
```

It is apparent that in both cases the difference in the number of edges between exact and approximate solution was exactly 3, which is the same. This is just a single example, but the situation was identical for every 2 graph we tested, which is also proved by the plots at the beginning of this section.

8.4   Comparison of approximate algorithms with and without sorted form
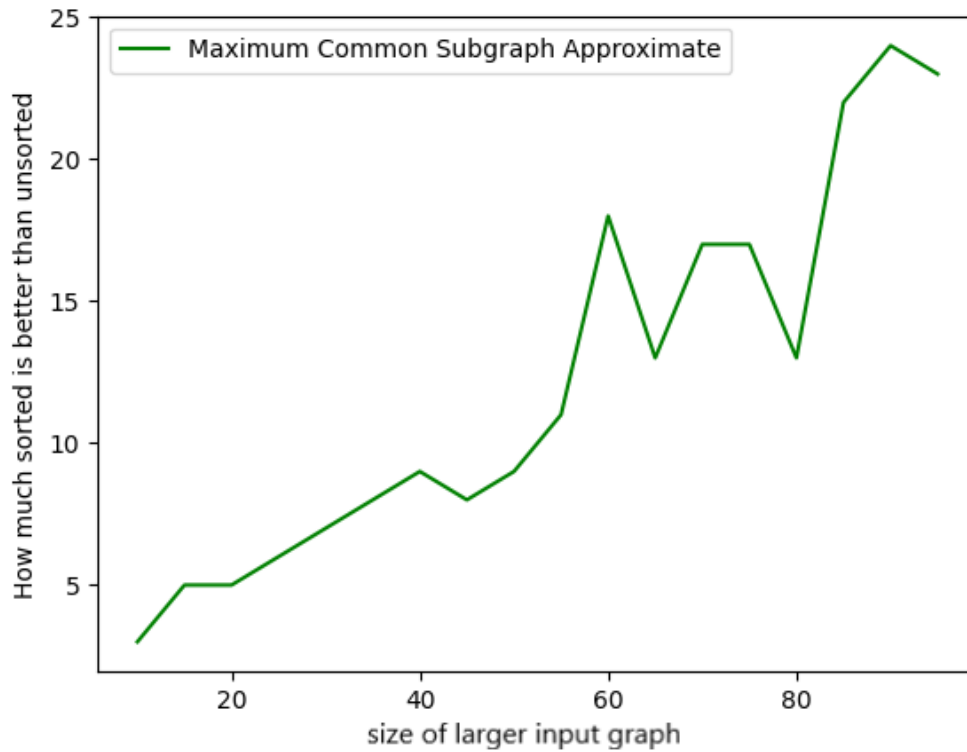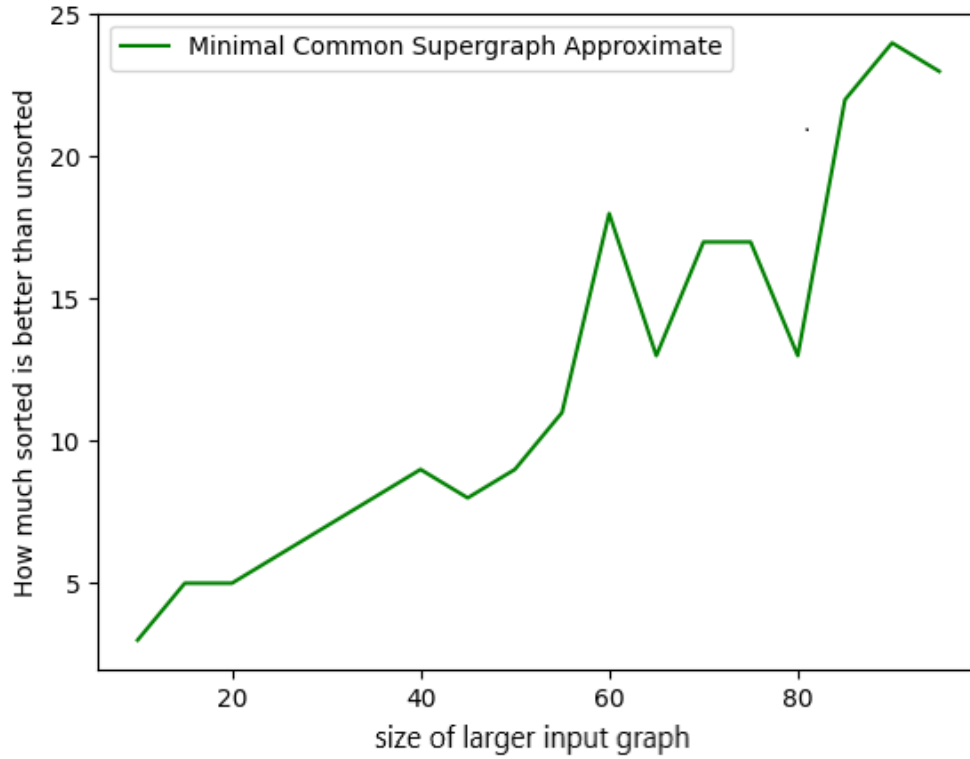
On this plots we can observe the difference between the number of edges in graph found by approximate algorithms which sort the input graph and the number of edges in graph found by approximate algorithms which do not sort the input graphs. It is apparent that the larger the input graph, the bigger effect the sorting has. In case of minimal common supergraph for graphs of 80 vertices the sorting version of algorithm found graphs with around 15 edges less than algorithm without sorting and in case of maximal common subgraph algorithm that is sorting the matrices found around 15 edges more than algorithm that do not sort the graphs. Which means that sorting the matrices makes the approximation much better especially for bigger graphs. It is worth remembering that using sorting in approximation algorithms does not affect the complexity. But the most interesting thing is that difference between algorithm which uses sorting and the one which does not is the same for both algorithms. Hence we have the same situation as for the difference in performance between the exact and approximate solutions.

8.5 Conclusions

From the presented observations we can conclude that finding exact solutions is very time consuming and almost impossible for very large graphs (at least with current technology). Even for small graphs with only 10 vertices it takes around 3 minutes to calculate the solution on a regular computer, so for larger graphs we have to approximate the solutions. To obtain a better approximation we decided to transform graphs into sorted versions. This procedure doesn't affect the complexity of the algorithm, but it allows us to get slightly better results. In our tests we discovered that this sorting improvement gets better as size of the graphs to which we apply algorithms gets larger.

9 Instruction

This project was implemented using $C\#$ programming language in Visual Studio, which is able to create an executable file with the program, so no additional software or environment is needed to run it. It is enough to double-click the executable in the provided EXE folder.
(NOTE: The executable was created in the 64-bit version to allow for more memory usage, thus it will not work on the 32-bit machines - in such case the appropriate executable should be compiled in Visual Studio after changing the compiler in project settings).
The program opens the console in which all steps are preceded by appropriate descriptions, thus the user should be able to use the software without problems. Commands to provide the input (for example specifying size of graphs to generate) should be accepted by pressing "Enter" key, but the rest of options runs immediately after choosing appropriate key.
At the beginning, the user can choose to run the algorithms on random graphs generated by the program or to provide their own input graphs from a file. In case of choosing the file input the user should type in the path of the file (e.g. "../Examples/test.txt"). The content of the file should have the following format:

5
0 1 1 0 0
0 0 1 0 1
0 0 0 1 0
0 0 0 0 1
0 0 0 0 0
4
0 1 1 0
0 0 0 0
0 1 0 0
0 1 0 0

Where:

1) first line contains the number of vertices (i.e. the size) of the first graph, let's say n.

2) lines second to $2 + n - 1$ contain the respective rows of first matrix, where each row is a sequence of 0's and 1's and each two digits in a row are separated by a single white space.

3) line $2 + n$ contains the number of vertices of the second graph, let's say k.

4) lines $2 + n + 1$ to $2 + n + k$ contain the respective rows of the second matrix, where each row is a sequence of 0's and 1's and each two digits in the row are separated by a single white space.

In case of choosing the random generation of graphs, the user is simply asked to specify the size of both input matrices - if at least one of the provided sizes will be more than 10, then only the approximate versions of the algorithms will be available. This is because the exact algorithms have exponential time complexity and even for graphs with only 10 vertices it takes around 3 minutes to find the solution.

NOTE: The *Source* folder contains a folder *AlgorithmsComputabilityProject* with all source files and code, and an .sln file which enables to run the solution in the Visual Studio IDE. If it is already installed on the computer, then a double-click on the .sln file would automatically launch the Visual Studio and enable to view all the source files in one place or even compile the project again.

9.1   Files naming convention

The final solution contains folder *Examples*, which consists of around 50 .txt files with exemplary pairs of matrices that can be used to test our program. All files have the format specified below, with larger matrix always listed as the first. Additionally, all graphs that are not isomorphic to their *pair* matrix or doesn't contain any subgraph isomorphic to their *pair* matrix, were generated randomly with 30% probability for choosing an edge (1). That is because, in graphs larger than 5 vertices the huge number of edges was making the output of the algorithms quite unreadable and we wanted to eliminate that effect by reducing the probability for choosing edges. All names of the provided exemplary files follow one of the three formats listed below:

- **x_x_iso** - two isomorphic graphs with the same number of vertices x.

- **x_y_noiso** - two randomly generated graphs, where the smaller graph is not isomorphic with any subgraph of the larger one. The graphs are of sizes x, y and $x \geq y$.

- **x_y_isosub** - two graphs with sizes x and y ($x > y$), where the smaller one is isomorphic to some subgraph of the larger graph.

10   Version list

Date	Version	Comment
28.10.2021	1.0	Sections 1-7 without complexity analysis
04.11.2021	1.1	Complexity analysis of the solution
23.11.2021	1.2	Section 8 - Results
24.11.2021	1.3	Conclusions and instructions
25.11.2021	1.4	Correction and version list
05.12.2021	1.5	Files naming convention
07.12.2021	2.0	Final correction