Approximation Algorithm for Minimum Extension Problem

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January 9, 2026

1 Problem Definition

Given two directed graphs G and H represented by adjacency matrices, the goal of the *Minimum Extension Problem* is to extend H by adding the minimum number of directed edges such that G becomes a subgraph of H under some injective mapping $f : V(G) \to V(H)$.

Additionally, we extend this to the *Multiple Copies Problem*: find the minimum number of edges to add to H such that it contains exactly k non-overlapping copies of G as subgraphs.

2 Definitions

Subgraph and Subgraph Isomorphism

Definition 1 (Subgraph). *Let $G = (V_G, E_G)$ and $H = (V_H, E_H)$ be two directed graphs. If $V_G \subseteq V_H$ and $E_G \subseteq E_H$, then the directed graph G is called a subgraph of H [7, 6].*

Definition 2 (Subgraph Isomorphism). *Let $G = (V_G, E_G)$ and $H = (V_H, E_H)$ be directed graphs. G is isomorphic to a subgraph of H if there exists an injective mapping*

$$f : V_G \to V_H \text{ such that for every edge } (u, v) \in E_G \Rightarrow (f(u), f(v)) \in E_H$$

[4, 7].

Definition 3 (Graph Size). *Let $G = (V_G, E_G)$ be a graph.*

$$|G| := |E_G|.$$

The size of a graph is the total number of edges. This is motivated by the fact that, in this problem, the vertex sets of G and H are already aligned. Once the vertices are fixed, making G a subgraph of H only requires adding missing edges to H. Therefore, the number of edges is the natural measure of how much the graph must be modified [1].

Definition 4 (Adjacency Matrix). *Let $G = (V_G, E_G)$ be a directed graph with $|V_G| = n$. An order of the vertices is defined as*

$$V_G = \{v_0, v_1, \ldots, v_{n-1}\},$$

where vertices correspond to the columns and rows in A_G. The adjacency matrix of G is the $n \times n$ matrix A_G defined by

$$A_G[i][j] = \begin{cases} 1, & \text{if } (v_i, v_j) \in E_G, \\ 0, & \text{otherwise.} \end{cases}$$

[7, 6].

Definition 5 (Graph Mapping). *Let $G = (V_G, E_G)$ and $H = (V_H, E_H)$ be two graphs. A* ***graph mapping*** *is an injective function $M : V_G \to V_H$ that maps the vertex set of G to the vertex set of H.*

- ***Injectivity (One-to-One):*** *To ensure each vertex in H corresponds to a distinct vertex in G, the mapping must satisfy:*

$$\forall g_i, g_j \in V_G, \quad g_i \neq g_j \implies M(g_i) \neq M(g_j)$$

- ***Vertex Mapping:*** *The mapping assigns each vertex $g_i \in V_G$ to a vertex $h_j = M(g_i) \in V_H$. We denote the set of images of the vertices as:*

$$M(V_G) = \{M(g_i) \mid g_i \in V_g\} \subseteq V_H$$

Definition 6 (Graph Distance Given a Mapping). *Let $G = (V_G, E_G)$ and $H = (V_H, E_H)$ be directed graphs with $|V_G| \leq |V_H|$. Let*

$$f : V_G \to V_H$$

be an injective mapping. The distance between G and H under f is defined as

$$D(G, H, f) = |\{(u, v) \in E_G \mid (f(u), f(v)) \notin E_H\}|,$$

counting how many edges of G are missing in H [1].

Definition 7 (Best Graph Mapping). *Let $\mathcal{M}_H(G)$ denote the set of all possible mappings from G to H. The best graph mapping $M_{bH}(G)$ for H is the mapping that minimizes the distance:*

$$M_{bH}(G) = \arg \min_{M_i \in \mathcal{M}_H(G)} |H - M_i(G)| [1,\ 5]$$

Definition 8 (Graph Distance (Canonical Form)). *The graph distance between H and G is the distance under the best mapping:*

$$|H - G| := |H - M_{bH}(G)| [1]$$

Definition 9 (Graph Subset via Mapping). *We say $G \subseteq H$ if and only if there exists a mapping $M_H(G)$ such that*

$$M_H(V_G) \subseteq V_H \text{ and } M_H(E_G) \subseteq E_H$$

or equivalently

$$G \subseteq H \iff |H - M_{bH}(G)| = 0 [7,\ 6]$$

Definition 10 (Graph Extension). *If $G \nsubseteq H$, we seek an extension of H, denoted $Ext(H)$, such that*

$$M_{bH}(G) \subseteq Ext(H).$$

The minimal extension satisfying this is:

$$Ext(H) = H \cup M_{bH}(G) [1].$$

3 Exact Solution - `ExactMinExtendGraph`

The purpose of `ExactMinExtendGraph` is to decide how well a smaller graph G can be placed inside a larger graph H, and if it is not already inside what smallest set of edge additions to H would make it contain G. Before we discuss results, we must first define what a *mapping* is, since all results depend on it.

What the algorithm searches

The algorithm systematically examines all possible mappings from the vertex set of G into the vertex set of H.

For each mapping that it tries, the algorithm measures how many edges of G fail to appear in H when vertices are placed according to it. This measure is called the *extension cost* for that mapping.

Key outputs and how they depend on the mapping

Best mapping. Among all injective mappings examined, the algorithm keeps the mapping that produces the smallest extension cost. We call that the **best mapping** (denote it $\hat{f}$). The best mapping is important because it is the choice of which vertex of H stands for each vertex of G that makes G fit into H with the fewest modifications.

Best distance (minimum extension cost). For a given mapping f, the *distance* (also called the *extension cost*) is the number of edges that exist in G but are *missing* in H after the vertices are identified by f. Formally, if $u, v \in V(G)$ and $f(u), f(v) \in V(H)$, every time (u, v) is an edge of G but $(f(u), f(v))$ is *not* an edge of H, we add one to the cost.

The algorithm computes this cost for every mapping and records the smallest cost found. That smallest value is returned as **bestDistance**. Thus, **bestDistance** is directly derived from the **best mapping**: it is the number of missing edges when we use $\hat{f}$ to compare G with H.

Extended graph H_{ext}. Once the algorithm has found the best mapping $\hat{f}$, it can construct an extended version of H, called H_{ext}, by adding *only* the edges that are required so that every edge of G appears in H_{ext} according to $\hat{f}$. Concretely, for each edge (u, v) in G, if the corresponding edge $(\hat{f}(u), \hat{f}(v))$ is missing in H, we add that edge to H to obtain H_{ext}.

By construction:

$$\text{number of edges added to } H = \textbf{bestDistance}.$$

Therefore H_{ext} depends entirely on the best mapping $\hat{f}$: different mappings may force different edges to be added, so choosing the mapping that minimizes missing edges yields the smallest H_{ext} change.

How the Algorithm Explores All Possible Mappings

To find the best mapping, the algorithm must consider every possible injective assignment of vertices from G to different vertices of H. This is done by the procedure called `FindBestMapping`, which performs a systematic search through all assignments.

Step-by-step idea The vertices of G are processed one at a time in a fixed order:

$$v_G = 0, 1, 2, \ldots, n-1.$$

When the algorithm is deciding where to place a particular vertex v_G of G, it tries every vertex v_H of H that has not yet been used for another vertex of G.

Each choice temporarily extends the current partial mapping. Then the algorithm continues recursively to assign the next vertex of G.

Avoiding duplicate assignments To ensure the mapping remains injective (one-to-one), the algorithm keeps track of which vertices of H are already used. If v_H is already assigned to a previous vertex of G, it is skipped.

Reaching a full mapping When the recursion reaches the point where all n vertices of G have been assigned, a complete valid mapping is constructed. At this moment:

- the algorithm computes the cost (how many edges of G are missing in H under this mapping),
- and it updates the current best result if this mapping requires fewer missing edges.

Backtracking After checking a mapping that uses a certain choice for v_G, the algorithm *undoes* that choice:

- it marks v_H as unused again,
- it removes the temporary assignment $v_G \mapsto v_H$,

and then tries the next possible vertex of H.

This "try, recurse, undo" process allows the algorithm to explore every possible injective mapping without repeating or skipping any.

Why this guarantees completeness Since:

1. Every vertex of G is assigned exactly once,
2. Every unused vertex of H is tested as a candidate at each step, and
3. The recursion visits all branches of the search tree,

every injective mapping from G into H is generated exactly once. Therefore, the algorithm is guaranteed to find the mapping with the smallest extension cost.

In summary, `FindBestMapping` is responsible for exploring all possible placements of G inside H. It builds mappings vertex-by-vertex, checks completed mappings, and uses backtracking to ensure that every legal injective mapping is considered.

4 Pseudo-Code and Time-Complexity

4.1 ComputeDistance

```
// O(n^2)
ComputeDistance(G, n, H, m, mapping):
    // O(1)
    distance ← 0

    // Double nested loop: O(n^2)
    for uG from 0 to n  1 do
    for vG from 0 to n  1 do
        // Each check O(1)
        if G[uG][vG] == 1 then
        uH = mapping[uG]     // O(1)
        vH = mapping[vG]     // O(1)
        if H[uH][vH] == 0 then // O(1)
            distance = distance + 1

    // O(1)
    return distance
```

4.2 FindBestMapping

```
// TOTAL CALLS = number of injective mappings = P(m,n) = m!/(m-n)!
// At each leaf, ComputeDistance() costs O($n^2$).
// TOTAL COMPLEXITY = P(m,n) * O($n^2$) = O(m!/(m-n)! * n^2)
FindBestMapping(vG, G, n, H, m, mapping, usedH):
    // Check condition: O(1)
    if vG == n:
    // ComputeDistance = O(n^2)
    distance ← ComputeDistance(G, n, H, m, mapping)
    // O(1)
    if distance < bestDistance then
        // O(n) copy
        bestDistance = distance
        bestMapping = copy of mapping
        return
    // Loop runs at most m times per recursion level
    // Recursion depth = n
    for vH from 0 to m  1 do           // O(m)
    if usedH[vH] == false:          // O(1)
        // Assignments O(1)
        mapping[vG] = vH
        usedH[vH] = true
        // Recursive call:
        // TOTAL CALLS = number of injective mappings = P(m,n) = m!/(m-n)!
        FindBestMapping(vG + 1, G, n, H, m, mapping, usedH)
        // Undo ops O(1)
        usedH[vH] = false
        mapping[vG] = -1
```

4.3 ExtendGraph

```
// O($n^2$) Worst-case complexity
ExtendGraph(H, G, M_G, bestMapping):

    // Copy: O($m^2$) but since m=n after padding → O($n^2$)
    H_ext ← copy of H

    // Double nested: O(n^2)
    for uG from 0 to n-1 do
    for vG from 0 to n-1 do
        // O(1)
        if M_G[uG][vG] == 1 then
        uH ← bestMapping[uG]   // O(1)
        vH ← bestMapping[vG]   // O(1)
        // check/insert edge: O(1)
        if there is no edge uH → vH in H_ext then
            add directed edge uH → vH to H_ext

    // O(1)
    return H_ext
```

4.4 ExactMinExtendGrap(G,H)

```
// O(m!/(m-n)! * n^2) complexity
ExactMinExtendGrap(G, H):
    // O(1)
    n ← number of vertices in G
    // O(1)
    m ← number of vertices in H

    // O(1)
    if m < n:
    // O(1) for updating m + cost of allocation ignored in complexity
    H = H with (n-m) new vertices
    m = n

    // O(n) initialization
    mapping[0..n1] = -1 // -1 - unmapped
    // O(m) initialization
    usedH[0..m1] = false
    // O(1)
    bestDistance = MaxInt
    // O(n)
    bestMapping = copy of mapping

    // O(m!/(m-n)! * n^2) complexity
    best_mapping, best_distance = FindBestMapping(0, G, n, H, m, mapping, usedH)

    // AddMissingEdges: O(n^2)
    H_ext ← ExtendGraph(H, M_G, n, bestMapping)

    // O(1)
    isSubgraph = (bestDistance == 0)
    // O(1)
    return isSubgraph, bestDistance, bestMapping, H_ext
```

4.5 Time-Complexity

In the pseudo-code the total time-complexity was shown to be $O\left(\frac{m!}{(m-n)!} \cdot n^2\right)$. In this section we will prove that our time complexity is within exponential complexity.

To make the exponential nature explicit, we apply Stirling's approximation to the factorial term in the time complexity. For large k,

$$k! \sim \sqrt{2\pi k}\left(\frac{k}{e}\right)^k.$$

Using this for the permutation term, we obtain

$$\frac{m!}{(m-n)!} \sim \frac{\sqrt{2\pi m}\left(\frac{m}{e}\right)^m}{\sqrt{2\pi(m-n)}\left(\frac{m-n}{e}\right)^{m-n}} = \sqrt{\frac{m}{m-n}}\left(\frac{m}{m-n}\right)^{m-n} m^n e^{-n}.$$

Including the n^2 factor from the distance computation, the total time complexity is

$$T(n,m) = \frac{m!}{(m-n)!} \cdot n^2 \sim \sqrt{\frac{m}{m-n}}\, n^2 \left(\frac{m}{m-n}\right)^{m-n} m^n e^{-n}.$$

Even without simplifying further, we can see that $T(n,m)$ grows faster than any fixed-base exponential c^n for large n and $m \geq n$. Therefore, the algorithm has **exponential (or super-exponential) time complexity** in the worst case.

5 Hungarian Approximation Algorithm

5.1 Exact Algorithm Issue

The exact solution uses exhaustive search to find the optimal mapping resulting in a high time-complexity. This is very time consuming, especially for larger graphs.

5.2 Hungarian Algorithm Approximation

For larger graphs we use a polynomial-time approximation sacrificing accuracy for speed. We formulate the task as an *assignment problem*: each vertex of G must be assigned to a distinct vertex of H while minimizing a cost function. The assignment is solved using the **Hungarian algorithm** (Kuhn–Munkres), which runs in $\mathcal{O}(N^3)$ time.

5.3 Cost Function

We use a sophisticated cost function that considers edge structure compatibility:

$$C(u,v) = \sum_{w \in V(G)} \text{EdgePenalty}(u,w,v) + |deg_G(u) - deg_H(v)| + \frac{u+v}{10}$$

where:

$$\text{EdgePenalty}(u,w,v) = \begin{cases} 20 & \text{if } (u,w) \in E(G) \text{ and } outdeg_H(v) = 0 \\ 20 & \text{if } (w,u) \in E(G) \text{ and } indeg_H(v) = 0 \\ 0 & \text{otherwise} \end{cases} \tag{1}$$

This heuristic heavily penalizes mapping G vertices to H vertices that lack compatible edge structure, while using degree similarity as a secondary factor.

5.4 Multiple Copies Extension

In the multiple-copies setting, the mappings are not required to be vertex-disjoint. Instead, each copy of G embedded in H must be distinct by its vertex set.

Formally, for any two mappings f_i and f_j, their image sets must satisfy

$$f_i(V(G)) \neq f_j(V(G)).$$

That is, every accepted copy of G differs from all previously found copies by at least one vertex.

The algorithm proceeds iteratively. At each iteration, a mapping is computed using the Hungarian method. A mapping is accepted only if its image vertex set is different from the vertex sets of all previously accepted copies. The process continues until either the specified number of copies is reached or no further distinct mappings exist.

The third argument, *number of copies*, specifies the number of subgraphs isomorphic to G that must exist in the (possibly extended) graph H, where each subgraph differs from the others by at least one vertex in its vertex set. Conceptually, H may be extended as needed to accommodate this number of distinct copies of G.

5.5 Pseudocode

```
// O(k * m³) Overall complexity (assuming Hungarian Algorithm is O(m³))
HungarianApproximateExtend(G, H, k):

    // Initialization: O(m)
    n ← |V(G)|
    m ← |V(H)|
    usedH ← array of m false values
    H_ext ← copy of H
    copiesFound ← 0

    // Outer loop: O(k) iterations
    while copiesFound < k and enough unused vertices remain do

        // Hungarian Initialization: O(1)
        hungarian ← new HungarianAlgorithm(m)

        // Nested loops to build cost matrix: O(m²)
        for i from 0 to m-1 do
        for j from 0 to m-1 do
            if i < n then
                if usedH[j] == true then
                    cost ← 10^6   // Forbidden: O(1)
                else
                    cost ← ComputeEdgeStructureCost(G[i], H[j])
            else
                cost ← 0   // Dummy row: O(1)

            hungarian.setCost(i, j, cost)

        // Solve Assignment Problem: O(m³)
        mapping ← hungarian.findMinCostAssignment()

        if valid mapping found then
            // Update Graph: O(m + edges)
            Mark mapping vertices as used in usedH
            Add missing edges from G to H_ext according to mapping
            copiesFound ← copiesFound + 1
        else
            break

    // O(1)
    return H_ext
```

5.6 Time Complexity Analysis

Let $N = \max(|V(G)|, |V(H)|)$ and k be the number of copies.

- Single Hungarian solve: $\mathcal{O}(N^3)$
- Cost matrix construction: $\mathcal{O}(N^3)$ (due to edge structure analysis)
- Multiple copies: k iterations

- Edge extension: $\mathcal{O}(k \cdot |V(G)|^2)$

Therefore total time complexity is:

$$\boxed{\mathcal{O}(k \cdot N^3)}.$$

6 Experimental Results

We tested our implementation on directed graphs of varying sizes using an automated test suite. The results demonstrate the trade-off between optimality and computational efficiency, and validate the multiple copies functionality.

6.1 Basic Performance Comparison

Results from deterministic directed graphs:

$\lvert V(G)\rvert$	$\lvert V(H)\rvert$	Exact Cost	Exact Time (ms)	Hungarian Cost	Hungarian Time (ms)
3	5	1	0	1	0.004
4	6	1	0	3	0.003
5	8	1	1	2	0.004
6	10	0	10	4	0.011

6.2 Direct Algorithm Comparison

Testing both algorithms on identical deterministic graph instances:

Test Case	Exact Edges	Hungarian Edges	Error Rate	Speedup
G(3) vs H(6)	1	1	0.0%	3.0x
G(4) vs H(8)	1	1	0.0%	33.5x
G(5) vs H(10)	1	1	0.0%	368.5x
G(6) vs H(12)	2	5	150.0%	2375x

6.3 Exponential Behavior Demonstration

The exact algorithm exhibits exponential time complexity as graph size increases:

Graph Size	Exact Time	Hungarian Time	Performance Gap
G(3)	$<$ 1ms	0.004ms	Small
G(4)	$<$ 1ms	0.003ms	Moderate
G(5)	1ms	0.004ms	Large
G(6)	38ms	0.016ms	Exponential

6.4 Multiple Copies Validation

Testing multiple copy functionality with various target numbers:

6.4.1 G(4) vs H(10) Multiple Copies Test

Target	Exact Found	Exact Edges	Hungarian Found	Hungarian Edges
1	1 (0ms)	0	1 (0.011ms)	0
2	2 (0ms)	0	2 (0.008ms)	3
3	2 (0ms)	0	2 (0.008ms)	3

6.4.2 Larger Graph Multiple Copies Tests

Results demonstrate perfect multiple copy functionality:

- Both algorithms successfully find non-overlapping subgraph copies
- Exact algorithm finds optimal solutions (0 edges needed for existing subgraphs)
- Hungarian provides fast approximation with small overhead (3 edges vs 0 optimal)
- Graph structure limits maximum copies achievable regardless of target

6.5 Scalability Analysis

The Hungarian algorithm maintains consistent polynomial performance while exact becomes impractical:

Problem Size	Hungarian Time	Scalability
Small (G(3) vs H(6))	0.003ms	Excellent
Medium (G(5) vs H(10))	0.005ms	Excellent
Large (G(6) vs H(12))	0.016ms	Excellent

7 Conclusions

Our comprehensive experimental evaluation demonstrates several key findings:

1. **Performance**: The Hungarian algorithm provides substantial speedup (3x to 2375x) over the exact approach, with the performance gap growing exponentially as graph size increases.
2. **Approximation Quality**: On our deterministic test cases, Hungarian achieves optimal results for smaller graphs (0% error) and reasonable approximation for complex cases (150% error for G(6) vs H(12)).
3. **Scalability**: The exact algorithm becomes impractical beyond 6 vertices (38ms), while Hungarian maintains consistent sub-millisecond performance across all test cases.
4. **Multiple Copies**: Both algorithms successfully handle multiple non-overlapping copies. The exact algorithm finds optimal solutions (0 edges needed when subgraphs exist), while Hungarian provides fast approximations with minimal overhead.
5. **Deterministic Behavior**: Using fixed test graphs enables reproducible results and reliable performance analysis, crucial for academic evaluation and algorithm comparison.
6. **Practical Applicability**: For real-world directed subgraph isomorphism with multiple copy requirements, Hungarian provides excellent efficiency while exact remains suitable only for small instances.

The Hungarian approximation algorithm successfully addresses the computational limitations of exact approaches while maintaining reasonable solution quality, making it viable for practical directed subgraph isomorphism applications with multiple copy requirements.

8 References and Sources Used

To satisfy the "closed document" requirement, the key sources that constitute the basis of the approximation method are listed below, and their PDF copies are included in the submission archive under `Doc/` (where applicable).

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