Novelty Assessment Report

Paper: Neural Graduated Assignment for Maximum Common Edge Subgraphs
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Abstract

The Maximum Common Edge Subgraph (MCES) problem is a crucial challenge with significant implications in domains such as biology and chemistry. Traditional approaches, which include transformations into max-clique and search-based algorithms, suffer from scalability issues when dealing with larger instances. This paper introduces ``Neural Graduated Assignment'' (NGA), a simple, scalable, unsupervised-training-based method that addresses these limitations. Central to NGA is stacking of differentiable assignment optimization with neural components, enabling high-dimensional parameterization of the matching process through a learnable temperature mechanism. We further theoretically analyze the learning dynamics of NGA, showing its design leads to fast convergence, better exploration-exploitation tradeoff, and ability to escape local optima. Extensive experiments across MCES computation, graph similarity estimation, and graph retrieval tasks reveal that NGA not only significantly improves computation time and scalability on large instances but also enhances performance compared to existing methodologies. The introduction of NGA marks a significant advancement in the computation of MCES and offers insights into other assignment problems. Code is open-sourced at https://anonymous.4open.science/r/NGA-10E3.

Core Task Landscape

This paper addresses: **Maximum Common Edge Subgraph Computation**

A total of **50 papers** were analyzed and organized into a taxonomy with **23 categories**.

Taxonomy Overview

The research landscape has been organized into the following main categories:

- **Exact Algorithms and Theoretical Foundations**
- **Approximate and Heuristic Methods**
- **Learning-Based and Neural Approaches**
- **Parallel and High-Performance Computing**
- **Problem Formulations and Mathematical Models**
- **Algorithmic Comparisons and Benchmarking**
- **Relationships to Other Graph Problems**
- **Applications in Molecular and Chemical Sciences**
- **Applications in Biological and Biomedical Domains**
- **Applications in Pattern Recognition and Data Mining**
- ... and 6 more categories

Complete Taxonomy Tree

- Maximum Common Edge Subgraph Computation Survey Taxonomy
- Exact Algorithms and Theoretical Foundations
  - Clique-Based Formulations (2 papers)
  - [3] On Finding All Connected Maximum-Sized Common Subgraphs in Multiple Labeled Graphs (Davoodi, 2025) View paper
  - [5] Enumerating all connected maximal common subgraphs in two graphs (Ina Koch, 2001) View paper
  - Branch-and-Bound and Search Tree Methods (3 papers)
  - [20] A branch&cut algorithm for the maximum common edge subgraph problem (G. Manic, 2009) View paper
  - [22] Fast Maximum Common Subgraph Search: A Redundancy-Reduced Backtracking Approach (Kaiqiang Yu, 2025) View paper
  - [23] The maximum common subgraph problem: Faster solutions via vertex cover (Faisal N. Abu-Khzam, 2007) View paper
  - Complexity and Hardness Results (2 papers)
  - [14] Improved Hardness of Maximum Common Subgraph Problems on Labeled Graphs of Bounded Treewidth and Bounded Degree (Tatsuya Akutsu, 2020) View paper
  - [21] On the approximability of the maximum common subgraph problem (Viggo Kann, 1992) View paper
  - Specialized Graph Classes (2 papers)
  - [8] Largest common subgraph of two forests (Rautenbach Dieter, 2024) View paper
  - [41] A Polynomial-Time Algorithm for Computing the Maximum Common Connected Edge Subgraph of Outerplanar Graphs of Bounded Degree (Tatsuya Akutsu, 2013) View paper
- Approximate and Heuristic Methods
  - Matching-Graph and Stable Core Approaches (2 papers)
  - [1] Fast approximate maximum common subgraph computation (Mathias Fuchs, 2025) View paper
  - [43] The Matching-Graph (Fuchs, 2024) View paper
  - Metaheuristic Optimization (2 papers)
  - [16] CytoMCS: a multiple maximum common subgraph detection tool for Cytoscape (Simon J. Larsen, 2017) View paper

- [25] A Simulated Annealing Algorithm for Maximum Common Edge Subgraph Detection in Biological Networks (Simon J. Larsen, 2016) View paper
- Learning-Based and Neural Approaches
  - Neural Search and Reinforcement Learning ★ (3 papers)
  - [0] Neural Graduated Assignment for Maximum Common Edge Subgraphs (Anon et al., 2026) View paper
  - [10] GLSearch: Maximum Common Subgraph Detection via Learning to Search (Yun-sheng Bai, 2020) View paper
  - [42] Learning to Search for Fast Maximum Common Subgraph Detection (Yun-sheng Bai, 2021) View paper
  - End-to-End Similarity and Retrieval (2 papers)
  - [7] Maximum Common Subgraph Guided Graph Retrieval: Late and Early Interaction Networks (Roy, 2022) View paper
  - [13] More Interpretable Graph Similarity Computation via Maximum Common Subgraph Inference (Zixun Lan, 2022) View paper
- Parallel and High-Performance Computing (3 papers)
  - [2] Parallel maximal common subgraphs with labels for molecular biology (Wilfried Agbeto, 2024) View paper
  - [24] Observations from Parallelising Three Maximum Common (Connected) Subgraph Algorithms (R. Hoffmann, 2018) View paper
  - [34] The Maximum Common Subgraph Problem: A Portfolio Approach (Quer, 2022) View paper
- Problem Formulations and Mathematical Models (2 papers)
  - [17] Formulations for the maximum common edge subgraph problem (Etienne de Gastines, 2023) View paper
  - [29] A poset metric from the directed maximum common edge subgraph (Robert R. Nerem, 2019) View paper
- Algorithmic Comparisons and Benchmarking (2 papers)
  - [11] A comparison of algorithms for maximum common subgraph on randomly connected graphs (H. Bunke, 2002) View paper
  - [28] A performance analysis on maximal common subgraph algorithms (Welling, 2011) View paper
- Relationships to Other Graph Problems (2 papers)
  - [6] Mean and maximum common subgraph of two graphs (H. Bunke, 2000) View paper
  - [26] On a relation between graph edit distance and maximum common subgraph (Bunke, 1997) View paper
- Applications in Molecular and Chemical Sciences
  - Molecular Similarity and Database Search (5 papers)
  - [12] Computing a maximum common edge subgraph of two molecular graphs (Prinz, n.d.) View paper
  - [15] Maximum common subgraph isomorphism algorithms and their applications in molecular science: a review (Hans-Christian Ehrlich, 2011) View paper
  - [19] Rascal: Calculation of graph similarity using maximum common edge subgraphs (J. W. Raymond, 2002) View paper
  - [30] Efficient maximum common subgraph (MCS) searching of large chemical databases (Roger A. Sayle, 2013) View paper
  - [32] Heuristics for Similarity Searching of Chemical Graphs Using a Maximum Common Edge Subgraph Algorithm (John W. Raymond, 2002) View paper
  - Clustering and Substructure Representation (2 papers)
  - [33] Improving graphs of cycles approach to structural similarity of molecules (Stefi Nouleho Ilemo, 2019) View paper
  - [36] Representing clusters using a maximum common edge substructure algorithm applied to reduced graphs and molecular graphs (Eleanor J. Gardiner, 2007) View paper
  - Reaction Analysis and Rule Inference (2 papers)
  - [31] Deep Graph Learning in Subgraph Matching and Retrosynthesis (Lan, 2024) View paper
  - [45] Automatic Inference of Graph Transformation Rules Using the Cyclic Nature of Chemical Reactions (Flamm, 2016) View paper
- Applications in Biological and Biomedical Domains (3 papers)
  - [4] Finding maximum common contractions between phylogenetic networks (Bertrand Marchand, 2025) View paper
  - [35] Finding recurrent RNA structural networks with fast maximal common subgraphs of edge-colored graphs. (Antoine SoulÃ©, 2021) View paper
  - [38] Quantum algorithm for identifying RNA 3D motifs by processing RNA secondary structure graphs (Jing-Kai Fang, 2025) View paper
- Applications in Pattern Recognition and Data Mining (3 papers)
  - [27] Effective feature construction by maximum common subgraph sampling (Leander Schietgat, 2011) View paper
  - [37] Mining minimal contrast subgraph patterns (Roger Ming Hieng Ting, 2006) View paper
  - [40] Maximum Common Sub-Graph Extraction (M Terra-Neves, 2019) View paper
- Applications in Network Analysis and Monitoring (2 papers)
  - [47] Performance monitoring of large communication networks using maximum common subgraphs (Vijayalakshmi Ramasamy, 2011) View paper
  - [49] A divisive clustering algorithm for performance monitoring of large networks using maximum common subgraphs (Vijayalakshmi Ramasamy, 2011) View paper
- Specialized Applications and Emerging Domains (3 papers)
  - [9] Coverage bias in small molecule machine learning (Fleming Kretschmer, 2025) View paper
  - [39] A Method for Matching Information of Substation Secondary Screen Cabinet Terminal Block Based on Artificial Intelligence (Weiguo Cao, 2024) View paper
  - [50] Value of graph topology in vascular biometrics (Arathi Arakala, 2017) View paper
- Connected Subgraph Variants (1 papers)
  - [18] Fast similar subgraph search with maximum common connected subgraph constraints (Huiqi Hu, 2013) View paper
- Software Tools and Implementations (1 papers)
  - [44] wi2trier/cbrkit: v0.26.2 (Mirko Lenz, 2025) View paper
- Alternative Computational Paradigms (1 papers)
  - [48] A DNA-based graph encoding scheme with its applications to graph isomorphism problems (S. Hsieh, 2008) View paper
- Context Analysis and Text Processing (1 papers)
  - [46] Word-Graph Construction Techniques for Context Analysis (Wu Jue, 2024) View paper

Narrative

Core task: maximum common edge subgraph computation. The field is organized around several complementary perspectives. Exact algorithms and theoretical foundations establish hardness results and provably optimal methods, while approximate and heuristic approaches trade guarantees for scalability on large instances. Learning-based and neural methods have emerged more recently, applying deep learning and reinforcement learning to guide search or directly predict subgraph correspondences. Parallel and high-performance computing branches address computational bottlenecks through distributed execution. Meanwhile, the taxonomy also

reflects diverse problem formulations—such as connected variants or edge-contraction models—and a rich landscape of applications spanning molecular sciences, biological network analysis, pattern recognition, and network monitoring. Works like MCS Algorithms Review[15] and MCES Formulations[17] help anchor the methodological and modeling diversity, while tools such as CytoMCS[16] illustrate practical software implementations.

Within the learning-based branch, a small but growing cluster explores neural search and reinforcement learning strategies that learn to navigate the combinatorial search space more efficiently than classical heuristics. GLSearch[10] and Learning to Search[42] exemplify efforts to train models that adaptively prune or prioritize candidate mappings. Neural Graduated Assignment[0] sits squarely in this line of work, employing a differentiable graduated assignment framework to iteratively refine correspondences via neural guidance. Compared to GLSearch[10], which focuses on learning search policies, Neural Graduated Assignment[0] emphasizes continuous relaxation and gradient-based optimization. This contrasts with purely discrete heuristics like those in Heuristics Chemical Graphs[32] or exact branch-and-cut methods such as Branch Cut MCES[20], highlighting an ongoing tension between interpretability, scalability, and solution quality as the community explores how neural architectures can complement or replace traditional combinatorial techniques.

Related Works in Same Category

The following **2 sibling papers** share the same taxonomy leaf node with the original paper:

1. GLSearch: Maximum Common Subgraph Detection via Learning to Search

Authors: Yun-sheng Bai, Derek Xu, Yunsheng Bai, Alex Wang, Ken Gu, et al. (10 authors total) | **Year/Venue**: 2020 • International Conference on Machine Learning | **URL**: View paper

Abstract

Detecting the Maximum Common Subgraph (MCS) between two input graphs is fundamental for applications in drug synthesis, malware detection, cloud computing, etc. However, MCS computation is NP-hard, and state-of-the-art MCS solvers rely on heuristic search algorithms which in practice cannot find good solution for large graph pairs given a limited computation budget. We propose GLSearch, a Graph Neural Network (GNN) based learning to search model. Our model is built upon the branch and bound algo...

Relationship Analysis

Both papers belong to the Neural Search and Reinforcement Learning category, employing GNN-based learning frameworks to guide the search for maximum common subgraphs. GLSearch uses a Deep Q-Network to select node pairs within a branch-and-bound algorithm for MCS computation, incorporating pre-training and imitation learning stages. In contrast, the original paper (NGA) formulates MCES as a Quadratic Assignment Problem on an Association Common Graph and uses learnable temperature parameters in a graduated assignment framework with unsupervised training, rather than reinforcement learning with node-pair selection heuristics.

2. Learning to Search for Fast Maximum Common Subgraph Detection

Authors: Yun-sheng Bai, Yunsheng Bai, Derek Xu, Yizhou Sun, Wei Wang | **Year/Venue**: 2021 | **URL**: View paper

Abstract

Detecting the Maximum Common Subgraph (MCS) between two input graphs is fundamental for applications in biomedical analysis, malware detection, cloud computing, etc. This is especially important in the task of drug design, where the successful extraction of common substructures in compounds can reduce the number of experiments needed to be conducted by humans. However, MCS computation is NP-hard, and state-of-the-art MCS solvers rely on heuristics in search which in practice cannot find good sol...

Relationship Analysis

Both papers belong to the Neural Search and Reinforcement Learning category, employing GNN-based learning frameworks to guide the search for maximum common subgraphs. GLSearch uses a Deep Q-Network to replace heuristics in a branch-and-bound algorithm (McSplit) for node pair selection, combining imitation learning with reinforcement learning to improve search efficiency. In contrast, the original paper (NGA) formulates MCES as a Quadratic Assignment Problem on an Association Common Graph and uses a differentiable graduated assignment process with learnable temperature parameters, operating in an unsupervised manner without requiring labeled training data or explicit search tree exploration.

Contributions Analysis

Overall novelty summary. The paper proposes Neural Graduated Assignment (NGA), a differentiable optimization framework combining neural components with graduated assignment for MCES computation. It resides in the 'Neural Search and Reinforcement Learning' leaf, which contains only three papers total, indicating a relatively sparse research direction within the broader taxonomy of fifty papers. This leaf sits under 'Learning-Based and Neural Approaches', distinguishing itself from exact algorithms, classical heuristics, and end-to-end similarity prediction methods that populate other branches of the field.

The taxonomy reveals that NGA's immediate neighbors include GLSearch and Learning to Search, both exploring neural guidance for combinatorial search. Broader context shows the field divides between exact methods (clique formulations, branch-and-bound), approximate heuristics (stable cores, metaheuristics), and emerging neural approaches. The 'Neural Search and Reinforcement Learning' scope explicitly focuses on GNN-based frameworks guiding search processes, while the sibling 'End-to-End Similarity and Retrieval' leaf addresses direct prediction tasks. NGA's graduated assignment approach positions it at the intersection of continuous optimization and discrete matching, diverging from purely discrete search policies.

Among seventeen candidates examined, the core NGA method shows one refutable candidate from four examined, while the unsupervised training framework (zero from six) and theoretical temperature analysis (zero from seven) appear less contested. The limited search scope—seventeen papers rather than hundreds—means these statistics reflect top semantic matches and citation neighbors, not exhaustive coverage. The graduated assignment mechanism and learnable temperature components appear more novel within this bounded sample, though the neural-guided search paradigm itself has established precedents in the examined literature.

Given the sparse three-paper leaf and modest seventeen-candidate search, NGA appears to occupy a relatively underexplored methodological niche combining continuous relaxation with neural parameterization. The analysis captures proximity to existing neural search work but cannot assess whether deeper literature contains closer antecedents. The theoretical contributions on temperature dynamics show no refutation among seven examined candidates, suggesting potential novelty within the sampled scope, though broader theoretical literature on graduated assignment remains outside this search boundary.

This paper presents **3 main contributions**, each analyzed against relevant prior work:

Contribution 1: Neural Graduated Assignment (NGA) method for MCES

Description: The authors introduce Neural Graduated Assignment (NGA), a novel neural-style algorithm that formulates MCES through Association Common Graph (ACG) construction and uses learnable temperature parameterization to approximate MCES solutions efficiently in polynomial time without exhaustive search.

This contribution was assessed against **4 related papers** from the literature. Papers with potential prior art are analyzed in detail with textual evidence; others receive brief assessments.

1. Drug repositioning by integrating known disease-gene and drug-target associations in a semi-supervised learning model

URL: View paper

Brief Assessment

Drug Repositioning Semi[58] applies semi-supervised learning with feed-forward perceptron neural networks and random forests to drug repositioning, not to solving MCES through neural-style algorithms with learnable temperature parameterization and Association Common Graph construction.

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2. Solving inexact graph isomorphism problems using neural networks

URL: View paper

Prior Art Analysis

Neural Inexact Isomorphism[59] demonstrates prior work on using neural networks to solve graph isomorphism problems through association graph construction. The candidate paper explicitly describes a neural network approach associated with an association graph for solving graph matching problems, which predates the ORIGINAL paper's claim of being the first to formulate MCES via Association Common Graph (ACG) construction with neural-style algorithms. Both papers employ the fundamental concept of constructing an association/common graph and applying neural network-based optimization, though they may target different specific problem variants.

Evidence

Evidence 1 - **Rationale**: The candidate paper presents a neural network approach for graph isomorphism problems, which encompasses MCES as a variant, predating the ORIGINAL's claim of being 'the first neural-style algorithm' for this problem class. - **Original**: we for the first time formulate the mces problem via the construction of an acg, and based on this formulation, we propose nga - the first neuralstyle algorithm to approximate the mces solution efficiently in polynomial time without relying on exhaustive exploration of the solution space - **Candidate**: we present a neural network approach to solve exact and inexact graph isomorphism

Evidence 2 - **Rationale**: Both papers use the concept of association graphs as the foundation for their neural network approaches. The candidate explicitly describes constructing an association graph and applying a neural network to it, which is the same core methodological framework claimed as novel in the ORIGINAL paper. - **Original**: to efficiently explore solutions of mces, we proposed to construct an acg, where compatible nodes and edges can be identified - **Candidate**: clique problem is associated with an association graph. a neural network n g associated with g

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3. A competitive winner-takes-all architecture for classification and pattern recognition of structures

URL: View paper

Brief Assessment

Winner Takes All[60] focuses on a competitive winner-takes-all architecture for classification and pattern recognition, not on neural algorithms for maximum common edge subgraph problems. The candidate's context mentions association graphs and maximum selectors but does not present a neural-style algorithm for MCES computation.

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4. A k-Winner-Takes-All Classifier for Structured Data

URL: View paper

Brief Assessment

k Winner Classifier[61] focuses on k-winner-takes-all networks for structured data classification, not on neural algorithms for maximum common edge subgraph problems or association common graph construction.

Contribution 2: Unsupervised training framework for MCES

Description: The method operates without requiring training data or supervision signals about the MCES itself (such as MCES structure or size), enabling efficient approximations when exact solutions are computationally infeasible.

This contribution was assessed against **6 related papers** from the literature. Papers with potential prior art are analyzed in detail with textual evidence; others receive brief assessments.

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1. Maximum Common Subgraph Matching

URL: View paper

Brief Assessment

Maximum Common Matching[63] focuses on image co-segmentation using maximum common subgraph computation, not on unsupervised training frameworks for MCES approximation. The candidate's context is too limited to assess novelty claims about training methodologies.

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2. The maximum common substructure as a molecular depiction in a supervised classification context: experiments in quantitative structure/biodegradability relationships

URL: View paper

Brief Assessment

Molecular Depiction Classification[66] focuses on supervised classification using MCS as a molecular descriptor for biodegradability prediction, not on unsupervised training methods for MCES approximation. The candidate requires labeled training data and supervision signals about compound activity, which directly contradicts the unsupervised nature claimed in the original contribution.

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3. Attributed graph mining and matching: An attempt to define and extract soft attributed patterns

URL: View paper

Brief Assessment

Attributed Graph Mining[65] focuses on soft attributed pattern extraction from attributed relational graphs without requiring MCES structure or size labels. However, it addresses a different problem domain (attributed graph pattern mining) rather than the maximum common edge subgraph problem that the original paper tackles.

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4. Graph Similarity Computation via Interpretable Neural Node Alignment

URL: View paper

Brief Assessment

Neural Node Alignment[64] focuses on graph similarity computation via node alignment for GED/MCS tasks, not on MCES approximation. The candidate does not demonstrate prior unsupervised MCES training methods.

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5. CS 231N Project Report Unsupervised learning of Visual Object Relations with Graph-Level Analogy

URL: View paper

Brief Assessment

Visual Object Relations[67] addresses unsupervised learning of visual relations in graph-structured scenes, not maximum common edge subgraph approximation. The candidate focuses on discovering visual object relations through graph-level analogy in image data, which is a fundamentally different problem domain from MCES computation.

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6. Semantic measure of plagiarism using a hierarchical graph model

URL: View paper

Brief Assessment

Semantic Plagiarism Measure[62] focuses on plagiarism detection using hierarchical graph models for semantic similarity, not on unsupervised methods for maximum common edge subgraph approximation. The candidate's context mentions 'unsupervised learning' and 'maximum common edge subgraph' only in passing, without describing any unsupervised training framework for MCES computation.

Contribution 3: Theoretical analysis of learnable temperature dynamics

Description: The authors provide theoretical analysis demonstrating how NGA's learnable temperature parameterization enables escaping local optima, achieves faster convergence through adaptive learning rates, and balances exploration-exploitation tradeoffs.

This contribution was assessed against **7 related papers** from the literature. Papers with potential prior art are analyzed in detail with textual evidence; others receive brief assessments.

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1. Cross-Graph Embedding With Trainable Proximity for Graph Alignment

URL: View paper

Brief Assessment

Cross Graph Embedding[55] focuses on trainable proximity parameters for graph alignment tasks, not on learnable temperature parameterization for optimization dynamics in assignment problems. The candidate does not address temperature-based annealing mechanisms or their theoretical properties.

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2. Annealed training for combinatorial optimization on graphs

URL: View paper

Brief Assessment

Annealed Training Graphs[51] focuses on annealed training for combinatorial optimization problems using temperature schedules, not graph matching with learnable temperature parameterization for MCES as in the original paper.

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3. Active Network Alignment: A Matching-Based Approach

URL: View paper

Brief Assessment

Active Network Alignment[53] focuses on active learning query strategies for network alignment using temperature parameters in Gibbs sampling, not on theoretical analysis of learnable temperature parameterization dynamics in graph matching optimization as proposed in the original paper.

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4. Learning critical temperature for homomorphic ARG matching by self-organising Hopfield network

URL: View paper

Brief Assessment

Critical Temperature Hopfield[57] focuses on self-organizing Hopfield networks for attributed relational graph (ARG) matching, not on learnable temperature parameterization in graph matching optimization or MCES problems. The candidate addresses a different problem domain and methodology.

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5. Matchings on infinite graphs

URL: View paper

Brief Assessment

Matchings Infinite Graphs[56] focuses on matching problems on infinite graphs using temperature parameters in Boltzmann-Gibbs distributions for graph matching, not on learnable temperature parameterization in neural optimization frameworks for graph matching as in the original paper.

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6. Adaptive simulated annealing: A near-optimal connection between sampling and counting

URL: View paper

Brief Assessment

Adaptive Simulated Annealing[54] focuses on adaptive cooling schedules for discrete partition functions in sampling/counting problems, not on learnable temperature parameterization in neural graph matching optimization. The temperature schedules are constructed algorithmically rather than learned through gradient descent.

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7. Dynamic Asymmetric Contrastive Learning with Adaptive Hard Negative Mining for Resume-Job Matching

URL: View paper

Brief Assessment

Dynamic Asymmetric Contrastive[52] focuses on resume-job matching with temperature parameters for contrastive learning, not graph matching optimization dynamics or graduated assignment frameworks.

Appendix: Text Similarity Detection

No high-similarity text segments were detected across any compared papers.

References

- [0] Neural Graduated Assignment for Maximum Common Edge Subgraphs View paper
- [1] Fast approximate maximum common subgraph computation View paper
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- [3] On Finding All Connected Maximum-Sized Common Subgraphs in Multiple Labeled Graphs View paper
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