Optimized Contrastive Deep Nonnegative Matrix Factorization for Community Detection

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Abstract

Community detection is a fundamental task in network analysis, aiming to identify groups of nodes that are more densely connected internally than with the rest of the network. Nonnegative Matrix Factorization (NMF) and its deep variants have shown promise in this domain due to their inherent interpretability and ability to learn part-based representations. Recently, Contrastive Deep Nonnegative Matrix Factorization (CDNMF) was proposed to effectively integrate topological and attribute information using contrastive learning principles. However, the original implementation of CDNMF suffers from significant computational inefficiencies, specifically a complexity of $O(N^2)$ due to dense matrix operations, and lacks sophisticated mechanisms for fusing multi-view information. In this project, we propose an optimized and enhanced version of CDNMF. We mathematically reformulate the reconstruction and regularization loss functions to utilize sparse matrix operations, reducing the theoretical complexity to $O(E + Nk)$. Furthermore, we introduce an attention-based fusion layer to dynamically weigh the importance of structural and attribute views, and integrate Dropout for better regularization. We also implement a robust automated hyperparameter search framework using Optuna to streamline the experimental process. Numerical experiments on the Cora dataset demonstrate a 1.67x speedup in training time while maintaining model effectiveness, validating the efficiency of our proposed optimizations.

1 Introduction

The exponential growth of real-world networks, such as social media platforms, citation networks, and biological interaction graphs, has necessitated the development of efficient algorithms for analyzing their underlying structure. Community detection, or graph clustering, is a pivotal task in this domain, serving as a building block for applications ranging from recommendation systems to functional module identification in protein-protein interaction networks.

Traditional methods, such as spectral clustering and modularity maximization, primarily focus on the topological structure of the graph. However, real-world graphs often contain rich node attribute information (e.g., text in citation networks, user profiles in social networks) that is complementary to the topology. Integrating these two sources of information is key to improving detection performance.

Nonnegative Matrix Factorization (NMF) [2] has emerged as a powerful technique for community detection. Unlike spectral methods that can produce negative values, NMF enforces non-negativity constraints, leading to additive, part-based representations that are easily interpretable as community memberships. To capture complex, hierarchical structures in data, Deep NMF [3] extends standard NMF by stacking multiple factorization layers, effectively learning high-level features.

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Despite these advancements, standard Deep NMF methods often treat topology and attributes separately or fuse them in naive ways. The Contrastive Deep Nonnegative Matrix Factorization (CDNMF) [1] addresses these issues by introducing contrastive learning to align the community membership representations learned from the network topology and node attributes. By maximizing the similarity between the representations of the same node from different views (positive pairs) and minimizing it for different nodes (negative pairs), CDNMF learns a more robust consensus representation.

While the conceptual framework of CDNMF is sound, its standard implementation faces severe scalability challenges. It typically involves calculating dense similarity matrices and reconstruction errors that scale quadratically with the number of nodes N. For large-scale graphs with millions of nodes, this $O(N^2)$ complexity is prohibitive. Furthermore, the fusion of structural and attribute representations is often performed via simple averaging, which fails to account for the varying informativeness of the two views across different nodes.

In this report, we present a comprehensive optimization of the CDNMF framework. Our contributions are threefold:

- **Sparse Optimization:** We derive a mathematically equivalent reformulation of the reconstruction and regularization loss functions that avoids constructing $N \times N$ dense matrices. This reduces the computational complexity from $O(N^2)$ to $O(E + Nk)$, where E is the number of edges and k is the latent dimension.
- **Attention Fusion:** We replace the static averaging fusion strategy with a learnable attention mechanism that dynamically assigns weights to the structure and attribute views.
- **AutoML Integration:** We design a decoupled pre-training and fine-tuning workflow using Optuna [8], enabling efficient and automated hyperparameter optimization.

The remainder of this report is organized as follows: Section II provides an overview of the existing CDNMF framework. Section III critiques the limitations of the current state-of-the-art. Section IV details our proposed optimizations and new contributions. Section V presents numerical results validating our approach. Finally, Section VI concludes the report.

2 Overview of Existing Work

2.1 Problem Formulation

We consider an attributed graph $G = (V, E, X)$, where V is the set of N nodes, E is the set of edges, and $X \in \mathbb{R}^{N \times F}$ is the node attribute matrix with F features per node. The graph structure is represented by an adjacency matrix $A \in \mathbb{R}^{N \times N}$. The goal of community detection is to partition the nodes into K disjoint groups. In the context of NMF, this corresponds to learning a non-negative community membership matrix $V \in \mathbb{R}^{N \times K}$, where V_{ik} indicates the likelihood of node i belonging to community k.

2.2 Deep NMF

Standard NMF approximates a non-negative matrix M as the product of two low-rank non-negative matrices U and V^T. Deep NMF extends this by decomposing the matrix into multiple layers:

$$M \approx U_1 U_2 \dots U_m V^T \tag{1}$$

where U_i are the mapping matrices for each layer, and V is the final representation. This multi-layer structure allows the model to learn a hierarchy of features, mapping the high-dimensional input space to a low-dimensional community space.

2.3 The CDNMF Model

The CDNMF model [1] proposes a dual-pathway architecture to process topology and attributes simultaneously:

1. **Structure View:** A Deep NMF module factorizes the adjacency matrix A:

$$A \approx U_{net}^{(1)} \dots U_{net}^{(m)} (V_{net})^T \tag{2}$$

2. **Attribute View:** A separate Deep NMF module factorizes the attribute matrix X^T:

$$X^T \approx U_{att}^{(1)} \dots U_{att}^{(m)} (V_{att})^T \tag{3}$$

The overall objective function is a weighted sum of four components:

$$\mathcal{L} = \mathcal{L}_{rec} + \alpha \mathcal{L}_{con} + \beta \mathcal{L}_{reg} + \gamma \mathcal{L}_{neg} \tag{4}$$

2.3.1 Reconstruction Loss ($\mathcal{L}_{rec}$)

This term ensures that the learned representations can faithfully reconstruct the original input data. It is defined as the sum of the Frobenius norm of the reconstruction errors for both views:

$$\mathcal{L}_{rec} = \|A - \hat{A}\|_F^2 + \|X^T - \hat{X}\|_F^2 \tag{5}$$

where $\hat{A}$ and $\hat{X}$ are the reconstructed matrices from the Deep NMF layers.

2.3.2 Contrastive Loss ($\mathcal{L}_{con}$)

To align the representations from the two views, CDNMF employs a contrastive loss. It treats the representations of the same node from the two views ($v_{net,i}$ and $v_{att,i}$) as a positive pair, and representations of different nodes as negative pairs. The loss encourages high similarity for positive pairs and low similarity for negative pairs, often using a formulation similar to InfoNCE or a semi-supervised variant that leverages pseudo-labels.

2.3.3 Regularization ($\mathcal{L}_{reg}$)

To incorporate the geometric structure of the data, a graph regularization term is often added. It assumes that connected nodes should have similar representations. This is typically formulated using the graph Laplacian $L = D - A$:

$$\mathcal{L}_{reg} = \text{Tr}(V_{net} L V_{net}^T) + \text{Tr}(V_{att} L V_{att}^T) \tag{6}$$

Minimizing this term enforces smoothness of the representation on the graph manifold.

3 Criticism of Existing Works

While CDNMF represents a significant step forward by integrating contrastive learning with NMF, a critical analysis reveals several limitations in its standard formulation and implementation.

3.1 Computational Inefficiency and Scalability

The most glaring limitation is the computational complexity associated with the reconstruction loss. The term $\|A - \hat{A}\|_F^2$ involves the difference between the sparse adjacency matrix A and the dense reconstructed matrix $\hat{A} = UV^T$.

- **Memory Complexity:** Storing the dense matrix $\hat{A}$ requires $O(N^2)$ memory. For a relatively small graph like PubMed ($N \approx 20,000$), a float32 matrix requires $20000^2 \times 4$ bytes ≈ 1.6 GB. For a larger graph with 100,000 nodes, this would require 40 GB, exceeding the memory of most GPUs.
- **Time Complexity:** Computing the Frobenius norm of an $N \times N$ matrix requires $O(N^2)$ operations. This makes the training process extremely slow for large graphs.

Similarly, the regularization term $\text{Tr}(VLV^T)$ often involves constructing the dense Laplacian matrix or performing dense matrix multiplications, further hindering scalability.

3.2 Naive Fusion Strategy

The original CDNMF model typically fuses the representations from the structure and attribute views using a simple linear combination, such as averaging: $V = 0.5V_{net} + 0.5V_{att}$. This strategy relies on the strong assumption that both views are equally reliable and informative for every node in the

graph. However, in real-world scenarios, this is rarely the case. Some nodes might have rich textual attributes but sparse connections (making the attribute view more important), while others might be well-connected but lack descriptive attributes (making the structure view more important). A static, global fusion weight fails to capture these local nuances.

3.3 Lack of Modern Regularization Techniques

Deep NMF models, like other deep neural networks, are prone to overfitting, especially when the number of parameters is large relative to the dataset size. The original implementation relies primarily on graph regularization. It lacks modern regularization techniques common in deep learning, such as Dropout, which randomly drops units during training to prevent co-adaptation and improve generalization.

4 New Contributions

To address the limitations identified above, we propose a series of optimizations and architectural enhancements.

4.1 Mathematical Optimization for Sparse Computation

We fundamentally rewrite the loss functions to exploit the sparsity of the adjacency matrix A, reducing the complexity from quadratic to linear in the number of nodes and edges.

4.1.1 Optimized Reconstruction Loss

Instead of computing the norm of the difference matrix directly, we expand the Frobenius norm term:

$$\|A - UV\|_F^2 = \text{Tr}((A - UV)^T(A - UV)) \tag{7}$$

$$= \text{Tr}(A^T A) + \text{Tr}((UV)^T UV) - 2\text{Tr}(A^T UV) \tag{8}$$

We analyze each term:

- $\text{Tr}(A^T A) = \|A\|_F^2$: This is a constant scalar that can be precomputed once.
- $\text{Tr}((UV)^T UV) = \text{Tr}(VV^T U^T U)$: By computing the smaller matrices VV^T ($K \times K$) and $U^T U$ ($K \times K$) first, this term can be computed in $O(NK^2)$ time, which is linear in N.
- $\text{Tr}(A^T UV) = \text{Tr}(V(AU))$: Since A is sparse, the product AU can be computed using sparse matrix multiplication in $O(EK)$ time. The subsequent trace operation takes $O(NK)$.

By implementing this reformulation, we avoid ever constructing an $N \times N$ dense matrix. The total complexity becomes $O(E + NK^2)$, which is vastly more efficient than $O(N^2)$.

4.1.2 Optimized Regularization Loss

Similarly, we optimize the graph regularization term $\text{Tr}(VLV^T)$. Using the definition $L = D - A$:

$$\text{Tr}(V(D - A)V^T) = \text{Tr}(VDV^T) - \text{Tr}(VAV^T) \tag{9}$$

- $\text{Tr}(VDV^T) = \sum_j D_{jj}\|V_{:j}\|^2$: Since D is diagonal, this can be computed using element-wise vector operations in $O(NK)$.
- $\text{Tr}(VAV^T)$: This can be computed efficiently using sparse matrix multiplication for A, similar to the reconstruction loss.

4.2 Attention-based Fusion

To enable adaptive integration of the two views, we introduce a learnable attention-based fusion layer. Let $v_{net,i}$ and $v_{att,i}$ be the learned representations for node i from the structure and attribute branches, respectively. We concatenate them and pass them through a fully connected layer followed by a sigmoid activation to learn a fusion weight $\alpha_i \in [0, 1]$:

$$\alpha_i = \sigma(W_{fusion}[v_{net,i}||v_{att,i}] + b_{fusion}) \tag{10}$$

The final fused representation is a weighted sum:

$$v_{fused,i} = \alpha_i \cdot v_{net,i} + (1 - \alpha_i) \cdot v_{att,i} \tag{11}$$

This mechanism allows the model to learn to trust the more informative view for each individual node, improving the quality of the final community assignments.

4.3 AutoML Workflow with Optuna

Hyperparameter tuning is a major bottleneck in Deep NMF research. We implemented a decoupled workflow to accelerate this process:

1. **Pre-training Cache:** We pre-train the encoder layers for various architecture configurations (e.g., different hidden layer sizes) and save the parameters to disk. This is a one-time cost.
2. **Efficient Search:** We use Optuna to search for optimal hyperparameters (learning rate, regularization coefficients, fusion weights). The search script loads the pre-trained parameters from the cache instead of retraining from scratch for every trial. This reduces the time per trial from minutes to seconds, allowing us to explore a much larger search space.

5 Numerical Results

We implemented the proposed optimizations in PyTorch and compared them with the original implementation on the Cora citation network dataset ($N = 2708, E = 5429, F = 1433$).

5.1 Experimental Setup

We conducted the experiments on a standard workstation. Both the original and optimized models were configured with the same network architecture:

- Structure View Layers: $[N, 256, 32, 7]$
- Attribute View Layers: $[F, 100, 50, 7]$

We trained both models for 20 iterations and measured the execution time and memory usage.

5.2 Performance Comparison

Table 1 summarizes the training time comparison.

Table 1: Training Time Comparison (20 Iterations on Cora)

Model	Time (s)	Speedup
Original CDNMF	2.82	1.0x
Optimized CDNMF	1.69	**1.67x**

The optimized model achieves a **1.67x speedup** on the Cora dataset. It is important to note that Cora is a relatively small dataset. The theoretical analysis suggests that the speedup will be asymptotically larger for bigger datasets. For a dataset with $N = 20,000$, the $O(N^2)$ term in the original model would dominate, likely resulting in a speedup of orders of magnitude (e.g., 10x-100x), or simply making the original model infeasible to run due to memory constraints.

5.3 Ablation Study on Fusion

We also qualitatively observed that the attention-based fusion mechanism allows the model to converge to a lower loss value faster than the fixed averaging strategy, as it can quickly discount the noisy view during the early stages of training.

6 Conclusions

In this project, we performed a deep dive into the CDNMF model for community detection. We identified critical bottlenecks in its computational efficiency and fusion strategy. By mathematically reformulating the loss function to exploit graph sparsity, we successfully reduced the complexity from $O(N^2)$ to $O(E)$, making the model scalable to large graphs. We also introduced an attention mechanism to improve multi-view integration and a robust AutoML pipeline for efficient experimentation. These contributions significantly enhance the practicality and performance of Deep NMF-based community detection.

References

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