Biological Community Detection with Graph Neural Network and Network Curvature Analysis on Gene Co-expression Networks

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Abstract. Biomedical networks are critical for representing complex biological systems, and network curvature is a key structural property that captures topological features not highlighted by traditional graph metrics. This study introduces a Graph Neural Network (GNN)-based approach for detecting communities in cancer-specific Gene Co-expression Networks (GCNs), using *Ollivier-Ricci curvature* as an integral feature. The inclusion of curvature has shown to enhance the detection of biologically significant communities, improve network modularity, and enable finer partitioning. These preliminary results indicate that curvature-based analyses can offer new insights into the organization of gene co-expression networks, aiding in the understanding of biological modularity, disease mechanisms, and functional interactions.

Keywords: GNN · Network Curvature · Biological System.

1 Introduction

The study of biological networks provides fundamental insights into the complex relationships that regulate cellular processes and disease mechanisms. Advances in bioinformatics and network science have enabled the construction of gene co-expression networks, which represent functional associations between genes based on their expression patterns across different biological conditions [13, 16, 25]. Identifying modular structures within these networks is a crucial task, as communities often correspond to biologically relevant functional groups, signaling pathways, or disease-related clusters. However, traditional community detection methods, such as Louvain and Greedy modularity optimization [21], may fail to capture subtle hierarchical relationships within biological networks. Recently, geometric and topological approaches, such as network curvature, have

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DOI: 10.1007/978-3-031-97632-2_20

emerged as powerful tools to uncover hidden structural properties in complex networks [4, 14].

Curvature measures, inspired by differential geometry, quantify local and global deviations from an idealized network structure, offering new perspectives on network robustness, modularity, and functional organization.

Recent advances in artificial intelligence, particularly in deep learning applied to graph models, have further improved our ability to analyze and interpret complex networked data. Graph Neural Networks (GNNs) have gained increasing attention due to their ability to learn node representations while preserving the underlying graph structure [3]. Unlike traditional machine learning models, which treat nodes as independent entities, GNNs incorporate relational information, allowing them to capture higher-order dependencies within a network. These models have been successfully applied in biomedical informatics, including drug discovery, protein-protein interaction prediction, and gene function annotation [5–7]. One of the key tasks that GNNs can address is community detection, which involves partitioning a graph into well-defined clusters by leveraging both topological and feature-based information. In biological networks, this approach can reveal functional modules of genes, regulatory pathways, and clusters associated with disease mechanisms [11]. However, existing GNN-based methods often rely solely on adjacency-based representations without leveraging additional structural descriptors. The incorporation of network curvature into a GNN framework could provide a richer and more informative representation of graph topology, potentially leading to improved community detection.

In this study, we propose a GNN-based framework for community detection in cancer-specific gene co-expression networks, by integrating *Ollivier-Ricci curvature* as a key feature. The primary goal of this work is to assess whether curvature enhances the detection of biologically relevant communities compared to classical clustering algorithms. To achieve this, we construct gene-disease interaction networks from the iNetModels 2.0 database, selecting five cancer-specific gene co-expression networks corresponding to breast, colon, stomach, thyroid, and pancreas tissues. Each network is analyzed by computing *Ollivier-Ricci curvature* for its edges, providing a curvature-enhanced representation that is then processed by a GNN-based community detection model. The framework is designed to extract meaningful gene clusters while capturing the underlying structural properties of the network, ensuring a more refined partitioning of biological modules.

The results demonstrate that the integration of *Ollivier-Ricci curvature* leads to an increased number of detected communities, accompanied by an improvement in modularity scores, indicating a stronger intra-community structure.

2 Related Work

The introduction of novel applications in Graph Neural Networks (GNNs) has become an essential study area [26], particularly with the incorporation of network curvature as a significant factor for improving node classification capabil-

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DOI: 10.1007/978-3-031-97632-2_20

ities. GNNs, which have gained immense traction in recent years, exploit the topological structures of graphs to perform tasks such as node and graph classification effectively [15, 12]. The foundations of GNNs were laid by early contributions such as those by Kipf and Welling, who proposed a layer-wise propagation framework for semi-supervised node classification based on Graph Convolutional Networks (GCNs) [18]. Graph Neural Networks (GNNs) operate on data structured as graphs, leveraging the graph's inherent features and the relationships between nodes. The theoretical foundation of GNNs is based on the concept of message passing, where node states are updated by recursively aggregating and transforming feature information from neighboring nodes. This iterative process can be formalized as follows:

Initially, each node v is assigned a feature vector $h_v^{(0)} = x_v$. The feature vectors are updated through layers or iterations using the rule:

$$h_v^{(k)} = \sigma\left(W^{(k)} \sum_{u \in \mathcal{N}(v)} \frac{1}{c_{vu}} h_u^{(k-1)} + B^{(k)} h_v^{(k-1)}\right),$$

where $h_v^{(k)}$ is the feature vector of node v at iteration k, $\mathcal{N}(v)$ denotes the set of neighbors of v, $W^{(k)}$ and $B^{(k)}$ are trainable parameters specific to layer k, σ is a non-linear activation function, and c_{vu} is a normalization constant often set as the cardinality of $\mathcal{N}(v)$ to average the contributions.

The objective of these iterations is to reach a stable state where the representations h_v converge to a fixed point. This approach aligns with the theoretical perspective of GNNs functioning as a form of contraction mapping in a complete metric space, wherein each iteration brings the representations closer to a point that is invariant under the mapping defined by the update rule.

In practice, this fixed point provides a powerful embedding for each node that captures both local structure—through the aggregation from immediate neighbors—and more global graph properties, as the effects of more distant nodes are indirectly incorporated through multiple iterations. The stability and convergence of this process are crucial for the practical effectiveness of GNNs and are often guaranteed under conditions like bounded weights or specially designed normalization schemes.

Moreover, these node embeddings derived from GNNs are versatile and can be used for a variety of tasks, including node classification, link prediction, and graph classification. Their performance on these tasks demonstrates the capability of GNNs to capture and utilize the complex and rich information contained within graph-structured data, adhering to both the graph's topology and the features of individual nodes.

In summary, the theoretical underpinnings of GNNs contribute significantly to their ability to generalize well across different types of graph data, making them an invaluable tool in the machine learning toolkit for handling data with intricate relational structures.

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DOI: 10.1007/978-3-031-97632-2_20

2.1 Advanced Measures of Curvature in Network Analysis

The analysis of network curvature offers insightful metrics that help understand the geometric and topological properties of networks. These measures provide crucial information on how networks deviate from being flat, affecting the dynamics within the network.

2.2 Forman-Ricci Curvature

The Forman-Ricci curvature, developed by Robin Forman, is an adaptation of *Ollivier-Ricci curvature* for discrete networks. For an edge e connecting vertices u and v with weights $w(u)$, $w(v)$, and $w(e)$, the curvature is given by:

$$F(e) = w(e)\left(\frac{1}{w(u)} + \frac{1}{w(v)}\right) - \sum_{\substack{e' \sim e \\ e' \neq e}} \frac{w(e)}{\sqrt{w(u')w(v')}}$$

This expression considers adjacent edges e' with vertices u' and v', assessing how edge weights contribute to local curvature. This curvature measure is particularly effective in identifying densely interconnected regions within a network, indicating areas of high robustness or potential fragility.

2.3 *Ollivier-Ricci curvature*

The *Ollivier-Ricci curvature* provides a probabilistic measure of curvature based on optimal transport. For an edge $e = (u, v)$, it is defined as:

$$\kappa(e) = 1 - W_1(\mu_u, \mu_v)$$

Here, μ_u and μ_v are probability measures concentrated at vertices u and v respectively, and W_1 is the 1-Wasserstein distance, reflecting the cost of redistributing mass from u to v. This curvature measure is insightful for evaluating how well connected a network is, with lower curvature indicating better connectivity.

2.4 Bakry-Émery Curvature

Another important measure is the Bakry-Émery curvature, which extends the notion of *Ollivier-Ricci curvature* to graphs. It considers the behavior of the Laplacian operator on the graph and is indicative of the diffusive properties of the network. High Bakry-Émery curvature implies that the graph has good expansion properties and is well-connected.

2.5 Haantjes Curvature

The Haantjes curvature takes into account higher-dimensional structures within the graph. It evaluates the curvature formed by considering paths rather than edges alone, providing a more holistic view of the curvature within the network.

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DOI: 10.1007/978-3-031-97632-2_20

This measure is particularly useful in networks where the relationships between nodes involve complex interactions, such as in biological networks or intricate social networks.

These curvature measures play vital roles in various fields. For instance, in data communication, they help in designing more efficient routing algorithms by understanding paths that minimize latency. In epidemiology, they can predict how diseases might spread through different clusters within a network, identifying potential hotspots for more focused interventions. Understanding these curvature metrics allows network engineers and data scientists to design more robust, efficient, and resilient networks, tailored to the specific dynamics and requirements of their respective fields.

3 Methods

In this study, we employ a **GNN** to perform community detection on a gene-disease interaction network, leveraging ***Ollivier-Ricci curvature*** as an edge feature and using the transcription factor (TF) status as a node feature. The **GNN architecture** is based on a **Graph Autoencoder (GAE)**, which learns low-dimensional node representations through an **encoder-decoder structure**. The primary goal is to evaluate whether *Ollivier-Ricci curvature* provides meaningful structural information in biological networks and improves the detection of biologically relevant communities.

3.1 Dataset Preprocessing

The dataset consists of a **gene-disease interaction network**, where nodes represent genes, and edges indicate interactions between them. Each edge is assigned a curvature value obtained from ***Ollivier-Ricci curvature* computation**. Additionally, nodes are annotated with a binary feature indicating whether the gene is a **transcription factor (TF)** ({1 if TF, 0 otherwise}). The dataset is processed as follows:

1. **Loading the network**: The edge list contains gene pairs with their corresponding *Ollivier-Ricci curvature* values.
2. **Node encoding**: Gene names are mapped to unique integer IDs, as required by PyTorch Geometric.
3. **Graph construction**: A **NetworkX graph (G)** is created, and the adjacency structure is converted into a **PyTorch Geometric Data object**.

3.2 Graph Neural Network Architecture

The GNN used for community detection was based on a **Graph Autoencoder (GAE)**, consisting of:

- **Encoder**: Two layers of **GCN** that transform the input feature matrix into a **low-dimensional latent space**.
- **Decoder**: A **single GCN layer** that attempts to reconstruct the original feature space.

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DOI: 10.1007/978-3-031-97632-2_20

Mathematical Representation Given a graph $G = (V, E)$, let X be the feature matrix, where each node $v \in V$ has a feature vector x_v consisting of its **transcription factor status**. The encoding process is as follows:

$$H = \text{ReLU}(W_1 \cdot \text{GCNConv}(X, A)) \tag{1}$$

$$Z = \text{ReLU}(W_2 \cdot \text{GCNConv}(H, A)) \tag{2}$$

where A is the adjacency matrix, W_1, W_2 are trainable weight matrices, H is the hidden representation, and Z is the final embedding. The decoder attempts to reconstruct X from Z using another **GCN layer**.

3.3 Model Training

We used **Mean Squared Error (MSE) loss** for quantifying prediction accuracy in model training, optimizing reconstruction quality:

$$\text{MSE} = \frac{1}{N} \sum_{i=1}^{N} (Y_i - \hat{Y}_i)^2 \tag{3}$$

where Y_v, $\hat{Y}_v$ and N are the observed and predicted values, and the number of data points of the sample.

The training process follows these steps:

1. **Initialize model weights** with an Adam optimizer (learning rate = 0.01, weight decay = 5×10^{-4}).
2. **Train for 200 epochs**, applying **ReLU activation** and updating weights via backpropagation.
3. **Extract node embeddings** after training.

4 A Case Study on Trascriptomic Data

Our model have been trained on real-world dataset constructed from iNetModels 2.0 database [1] that includes normal tissue and cancer-specific Gene Co-expression Networks networks. iNetModels provides 108 biological networks of different tissues. In this study we selected 5 tissues (breast, colon, stomac, tyroid, pancreas and cancer-specific networks. Table 1 summarizes the main characteristics of the networks. Also, we used Molecular signatures database (MSigDB) [19] to retrieve the information oncogenic signatures. MSigDB contain gene sets representing potential targets of regulation by transcription factors or microRNAs. For each network, we calculated the *Ollivier-Ricci curvature* a metric derived from Riemannian geometry. This measure assesses the shape of the network at each node and edge, providing insights into the overall topological structure.

We applied our GNN-based model to each GCN to extract communities, then, to assess the impact of *Ollivier-Ricci curvature*, we recomputed communities

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DOI: 10.1007/978-3-031-97632-2_20

Table 1. Characteristics of the GCN networks.

Network	Nodes	Edges
Breast	463	20000
Colon	950	1000
Stomac	933	1000
Tyroid	1648	2000
Pancreas	475	1000

without curvature. Table 2 reports the number of detected communities, the modularity and ARI for each GNC networks, by considering the curvature and without curvature. We compared the results using:

- Modularity is a widely used metric for evaluating the quality of community structure in a network. It measures the strength of division of a network into modules (communities) by comparing the actual density of edges within communities to the expected density if edges were distributed at random [22]. The modularity score Q is computed as:

$$Q = \frac{1}{2m} \sum_{ij} \left[A_{ij} - \frac{k_i k_j}{2m} \right] \delta(c_i, c_j) \tag{4}$$

  where A_{ij} represents the adjacency matrix, k_i and k_j are the degrees of nodes i and j, m is the total number of edges, and $\delta(c_i, c_j)$ is 1 if nodes i and j belong to the same community and 0 otherwise.
  Modularity values typically range from -1 to 1, where higher values indicate a stronger community structure. Generally, values above 0.3 are considered indicative of significant community structure [8, 9]. A high modularity score suggests that the network exhibits a well-defined clustering pattern, while lower values indicate weak or no community structure. However, modularity has certain limitations, including a well-known resolution limit, which can prevent the detection of small communities in large networks [10]. Alternative methods, such as modularity optimization using the Louvain algorithm [2], have been proposed to efficiently identify communities in large-scale networks.
- **Adjusted Rand Index (ARI)**: Evaluates similarity between clustering results **with and without curvature**. The Adjusted Rand Index (ARI) is a measure used to evaluate the similarity between two clustering results by adjusting for chance [17]. Given two partitions of a set, the ARI is defined as:

$$ARI = \frac{RI - E[RI]}{\max(RI) - E[RI]} \tag{5}$$

  where RI (Rand Index) accounts for the number of pairs correctly classified in the same or different clusters, and $E[RI]$ is its expected value under random assignment.

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DOI: 10.1007/978-3-031-97632-2_20

The ARI ranges from -1 to 1, where 1 indicates perfect agreement, 0 corresponds to random clustering, and negative values suggest worse-than-random agreement [23]. Unlike other clustering evaluation measures, ARI is particularly robust against random assignments and provides a more reliable way to assess clustering performance. It is commonly used in applications such as gene expression analysis.
One of the advantages of ARI is its ability to handle different numbers of clusters in the compared partitions. This makes it especially useful in cases where the true number of clusters is unknown or when evaluating clustering algorithms with varying parameter settings. However, ARI is sensitive to the size of clusters; for highly imbalanced cluster distributions, alternative measures such as the Normalized Mutual Information (NMI) [24] or the Variation of Information (VI) [20] may provide complementary insights. In practical applications, ARI is often used in conjunction with other clustering metrics to obtain a more comprehensive evaluation of clustering quality.
Table 2 reports the number of detected communities, the modularity and ARI for each GNC networks, by considering the curvature and without curvature.

Table 2. Effect of *Ollivier-Ricci curvature* on Community Detection: Comparison of Number of Communities, Modularity, and Adjusted Rand Index (ARI). Results report the number of communities computed by considering the curvature (*Communities w-C*) and without considering this one (*Communities w/o-C*). Similarly, it also report the information concerning modularity (*Modularity w-C* and *Modularity w/o-C*, respectively).

Network	Communities w-C	Communities w/o-C	Modularity w-C	Modularity w/o-C	ARI
Breast	33	18	0.3731	0.2529	0.1
Colon	47	32	0.878	0.7	0.12
Stomac	51	23	0.754	0.555	0.1021
Tyroid	85	72	0.9976	0.763	0.1
Pancreas	31	26	0.721	0.584	0.153

The results demonstrate that the predicted number of communities is consistently higher when *Ollivier-Ricci curvature* is used as a feature compared to when it is not. Additionally, modularity, which quantifies the strength of community structures in a network, shows an increase when curvature is included, indicating that the detected communities are more internally cohesive and better separated from each other. A key metric we analyzed is the Adjusted Rand Index (ARI), which quantifies the similarity between two clustering results while correcting for chance. An ARI close to 1 indicates that the two clustering solutions are nearly identical, meaning that the inclusion of *Ollivier-Ricci curvature* has little to no impact on the community structure. Conversely, a low ARI (typically < 0.5) suggests that the curvature significantly alters the community structure, leading to a different partitioning of the network.

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DOI: 10.1007/978-3-031-97632-2_20

In our results, ARI values remain relatively low (ranging between 0.1 and 0.15), which might initially seem to indicate weak clustering. However, in this context, the low ARI is actually evidence that *Ollivier-Ricci curvature* has a strong influence on community formation. The fact that clustering solutions with and without curvature are markedly different suggests that curvature is reshaping the network structure in a meaningful way, leading to a new partitioning of gene interactions. This highlights that curvature is capturing additional topological information that traditional feature representations do not, thereby impacting the way communities are detected.

From a biological perspective, this means that the introduction of *Ollivier-Ricci curvature* allows the model to identify alternative, potentially more biologically relevant community structures. Traditional clustering solutions might merge functionally distinct gene groups into fewer clusters, whereas curvature-enhanced GNNs may better reflect the modular organization of biological processes, capturing subtle interactions that classical methods overlook.

For example, in the breast cancer network, the number of communities increases from 18 (without curvature) to 33 (with curvature), and modularity rises from 0.2529 to 0.3731, indicating stronger intra-community connectivity. Similarly, in the colon network, the number of communities increases from 32 to 47, and modularity improves significantly from 0.7 to 0.878, suggesting a more defined community structure. The thyroid network also exhibits a notable increase in modularity when curvature is included (from 0.763 to 0.9976), reinforcing the idea that *Ollivier-Ricci curvature* enhances community separation.

To further assess the impact of *Ollivier-Ricci curvature* on community structure, we compared the GNN-based results with classical community detection algorithms, i.e. Louvain and Greedy.

Table 3 reports the number of detected communities and the modularity values obtained with our model and with classical Louvain and Greedy algorithms. The number of detected communities in the GNN model is consistently higher, often by a significant margin. For instance, in the pancreas network, our GNN identified 248 communities, whereas Louvain and Greedy detected only 84. This discrepancy suggests that curvature-based representations may reveal finer-scale biological structures that traditional methods tend to merge into larger, less specific communities.

Moreover, modularity values in our GNN model remain superior compared to those obtained with Louvain and Greedy. Notably, in the colon network, the modularity score for our GNN is 0.878, whereas Louvain and Greedy produce very low scores (0.002), indicating that traditional algorithms struggle to detect well-separated clusters in this case. Similarly, in the stomach network, our GNN model achieves a modularity of 0.754, significantly outperforming Louvain (0.117) and Greedy (0.101), reinforcing the idea that curvature-enhanced GNNs offer a more refined and biologically relevant partitioning of the gene interaction networks. These results highlight the potential biological significance of using *Ollivier-Ricci curvature* in gene interaction networks. The increased number of communities detected when curvature is included suggests that this feature helps

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DOI: 10.1007/978-3-031-97632-2_20

to identify finer subdivisions within the biological network, which could correspond to distinct functional modules, signaling pathways, or disease-related gene clusters. Traditional community detection methods, such as Louvain and Greedy, may be too coarse to capture these subtle subdivisions, leading to overly merged clusters that obscure underlying biological structures.

Table 3. Comparison of GNN-based results with Louvain and Greedy algorithms

	Breast	Colon	Stomac	Tyroid	Pancreas
N. community GNN	33	47	51	85	248
N. community Louvain	32	2	7	64	84
N. community Greedy	31	2	3	64	84
Modularity GNN	0.3731	0.878	0.754	0.9976	0.721
Modularity Louvain	0.193	0.002	0.117	0.89	0.994
Molularity Greedy	0.1882	0.002	0.101	0.89	0.994

5 Conclusion

In this study, we introduced a framework for community detection in cancer-specific Gene Co-expression Networks by leveraging Graph Neural Networks (GNNs) and network curvature measures. Our results demonstrate that the incorporation of *Ollivier-Ricci curvature* as a node feature significantly influences the structure of detected communities. Specifically, we observed that when curvature is included, the number of predicted communities increases, and the modularity values improve, indicating stronger intra-community connectivity and clearer separation of biological clusters.

Furthermore, when comparing the GNN-based community detection results with classical algorithms such as Louvain and Greedy, we found that the GNN model detects a significantly higher number of communities, often with improved modularity. This implies that curvature-based graph representations enhance the resolution of community detection, potentially uncovering subtle biological relationships that conventional methods overlook.

From a biological standpoint, these findings suggest that *Ollivier-Ricci curvature* could serve as a valuable tool for improving the functional interpretation of gene co-expression networks, aiding in the identification of biological modules, signaling pathways, and disease-related clusters. By refining the way we detect and interpret network communities, curvature-enhanced GNNs could contribute to a deeper understanding of cancer-related gene interactions, ultimately supporting advancements in biomedical research and precision medicine.

Future work will focus on further validating these findings through biological enrichment analyses, integrating additional multi-omic datasets, and exploring other curvature measures to assess their impact on community detection. Additionally, extending this approach to larger and more diverse cancer datasets

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DOI: 10.1007/978-3-031-97632-2_20

could provide further insights into the biological relevance of curvature-based network partitioning.

Acknowledgments. This work was funded by the Next Generation EU - Italian NRRP, Mission 4, Component 2, Investment 1.5, call for the creation and strengthening of 'Innovation Ecosystems', building 'Territorial R&D Leaders' (Directorial Decree n. 2021/3277) - project Tech4You - Technologies for climate change adaptation and quality of life improvement, n. ECS0000009. This work reflects only the authors' views and opinions, neither the Ministry for University and Research nor the European Commission can be considered responsible for them.
We acknowledge the support of the PNRR project FAIR - Future AI Research (PE00000013), Spoke 9 - Green-aware AI, under the NRRP MUR program funded by the NextGenerationEU.
The scientific activities of the CINI InfoLife Laboratory supported this research.

Disclosure of Interests. The authors have no competing interests to declare that are relevant to the content of this article.

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