A Review of Graph Neural Networks in Epidemic Modeling

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Abstract

Since the onset of the COVID-19 pandemic, there has been a growing interest in studying epidemiological models. Traditional mechanistic models mathematically describe the transmission mechanisms of infectious diseases. However, they often fall short when confronted with the growing challenges of today. Consequently, Graph Neural Networks (GNNs) have emerged as a progressively popular tool in epidemic research. In this paper, we endeavor to furnish a comprehensive review of GNNs in epidemic tasks and highlight potential future directions. To accomplish this objective, we introduce hierarchical taxonomies for both epidemic tasks and methodologies, offering a trajectory of development within this domain. For epidemic tasks, we establish a taxonomy akin to those typically employed within the epidemic domain. For methodology, we categorize existing work into *Neural Models* and *Hybrid Models*. Following this, we perform an exhaustive and systematic examination of the methodologies, encompassing both the tasks and their technical details. Furthermore, we discuss the limitations of existing methods from diverse perspectives and systematically propose future research directions. This survey aims to bridge literature gaps and promote the progression of this promising field. We hope that it will facilitate synergies between the communities of GNNs and epidemiology, and contribute to their collective progress.

CCS Concepts

• **Computing methodologies** → **Artificial intelligence**.

Keywords

Epidemiology; Graph Neural Networks; Spatial-Temporal Graphs

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1 Introduction

Epidemiology has long been a critical field, with its origins tracing back to ancient societies that observed patterns of disease spread [1, 2]. Although the conceptualization of epidemiology has evolved over time, the terms *health* and *control* have been predominantly associated with it since 1978 [3]. Currently, the World Health Organization (WHO) describes epidemiology as the investigation into the distribution and determinants of health-related states or events, encompassing issues including disease transmission, vaccination efforts [4, 5], cancer and diabetes treatment, etc. This definition underscores the field's emphasis on controlling health-related issues and making informed decisions.

To address a range of health-related challenges, there is an indispensable need for epidemic modeling, and researchers have devised various mechanistic models [6, 7]. These models, grounded in mathematical formulations, simulate the dissemination of infectious diseases by incorporating biological and behavioral underpinnings. By considering factors such as population, they yield insights into patterns of disease transmission and the efficacy of intervention strategies, thereby shaping public health policies [8, 9]. However, these knowledge-driven methods often depend on oversimplified or fixed assumptions that can lead to biases in modeling. Consequently, this compromises both the accuracy of predictions and their ability to generalize across different contexts.

To overcome the limitations of mechanistic models, there is an emerging trend to adopt data-driven approaches in epidemic forecasting tasks, with a particular emphasis on machine learning and deep learning models [10]. Specifically, Convolutional Neural Networks (CNNs) and Recurrent Neural Networks (RNNs) have demonstrated great success in various epidemiological predictive tasks, including forecasting daily new case counts, estimating virus reproduction and doubling times, and determining disease-related factors [11, 12, 13]. Despite their effectiveness in these tasks, these models often fall short in incorporating relational information from critical epidemiological data sources such as human mobility, geographic connections, and contact tracing. This deficiency restricts their utility in broader epidemiological applications.

Recently, the advances in Graph Neural Networks (GNNs) [14, 15, 16, 17] have set the stage for overcoming the aforementioned challenges in epidemic modeling. Specifically, GNNs stand out for

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their ability to aggregate diverse information through a message-passing mechanism, making them particularly suited for capturing relational dynamics within graphs [18, 19]. Thus, by representing interactions between entities as graphs, researchers can leverage GNNs to harness relational data effectively and facilitate epidemiology tasks [20, 21]. For instance, GNNs are often utilized to model spatial interactions [22] and other complex interactions [23], enhancing the analysis of graph data and yielding more precise predictions. In addition, GNNs bring a certain level of interpretability by quantifying the influence of individual nodes (or entities) on final prediction [24]. Moreover, the flexible design of GNNs facilitates their integration with traditional mechanistic and probabilistic models to leverage expert knowledge and offer measures of uncertainty. As a result, GNNs have found extensive applications in various tasks within the field including infection prediction [25] , outbreak source detection [26], intervention modeling [27], etc., facilitating advancements in epidemiology research.

Contributions. Given the pivotal role of epidemic modeling and the growing use of GNNs, a systematic review of these algorithms is vital for advancing the field. This paper aims to bridge the gap with an in-depth overview and categorization of GNN applications in epidemiology. Our objective is not just to spotlight current research but also to identify future research avenues, enriching the GNN and epidemiology fields. By categorizing tasks, summarizing methodologies, and suggesting future directions, we hope to support researchers venturing into this interdisciplinary area.

Connection to Existing Surveys. Unlike earlier surveys focusing on epidemiology and deep learning, which mainly predict COVID-19 outcomes and seldom cover GNN-based methods [10, 28, 29, 12], our paper provides an in-depth overview of GNNs in epidemic modeling. Previous studies have incorporated GNNs but often in limited contexts [30, 13], mostly virus transmission tasks. Our research, uniquely focused on GNN approaches, spans a wider array of epidemic modeling tasks and presents the most current review of GNN applications, delivering deeper insights than existing literature.

2 preliminaries and definitions

2.1 Learning on Graph Data

In this paper, we define the graph data as $G = (V, \mathcal{E})$, with V representing the node set comprising $|V| = N$ nodes. The edge set $\mathcal{E} \subseteq V \times V$ represents the connections between nodes. The feature matrix $\mathbf{X} = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N\}^\top \in \mathbb{R}^{N \times D}$ includes feature vectors $\mathbf{x}_i$ associated with node v_i, where D denotes the feature dimension. The adjacency matrix of G, denoted by $\mathbf{A} \in \mathbb{R}^{N \times N}$, sets $\mathbf{A}_{ij} = 1$ for any existing edge $e_{i,j} \in \mathcal{E}$ and $\mathbf{A}_{ij} = 0$ otherwise. The normalized adjacency matrix is given by $\hat{\mathbf{A}} = \mathbf{D}^{-1/2}\mathbf{A}\mathbf{D}^{-1/2}$. The degree matrix $\mathbf{D}$, being a diagonal matrix, is characterized by $\mathbf{D}_{i,i} = \sum_j \mathbf{A}_{i,j}$.

In the domain of graph learning, the node-level task stands out as a significant area of focus. The objective of this task is to forecast the properties (*i.e.*, numerical value or probability) or class of the individual nodes. This process entails training a neural network model that utilizes a subset of nodes with known properties, denoted as $\mathcal{V}_L$, to infer the properties of other unknown nodes. The essence of this training is encapsulated by optimizing the function:

$$\min_\theta \mathcal{L}(f_\theta(G)) = \sum_{v_i \in \mathcal{V}_L} \ell(f_\theta(\mathbf{X}, \mathbf{A})_i; y_i), \tag{1}$$

where the function $f_\theta(\mathbf{X}, \mathbf{A})$ aims to forecast the property for each node, with y_i representing the actual state of node v_i. The discrepancy between the predicted and true properties is quantified using a loss function $\ell(\cdot, \cdot)$, such as RMSE (Root Mean Square Error).

Over recent years, GNNs have garnered increasing interest and have been deployed across diverse fields, including bioinformatics, material science, chemistry, and neuroscience [31, 32, 33, 34]. Among them, Graph Convolutional Networks (GCN) [15] and Graph Attention Networks (GAT) [16, 17], have advanced the frontier of research on graph-structured data with their sophisticated and effective designs [14, 35, 36]. Typically, GNNs aim to learn graph representations, including node embeddings $\mathbf{h}_i \in \mathbb{R}^d$, by utilizing both the structural and feature information of a graph G. The process within a GNN involves two key operations: message passing and aggregation of neighborhood information. This involves each node in the graph repeatedly collecting and integrating information from its neighbors as well as its own attributes to enhance its representation. An L layers GNN can be described as:

$$\mathbf{h}_i^{(l+1)} = \sigma(\mathbf{h}_i^{(l)}, \mathrm{AGG}(\mathbf{h}_j^{(l)}; j \in \mathbf{A}_i)), \forall l \in [L], \tag{2}$$

where $\mathbf{h}_i^{(l)}$ denotes node v_i representation at layer l, starting with $\mathbf{h}_i^{(0)} = \mathbf{x}_i$ as initial features. $\mathbf{A}_i$ is node v_i's neighbors, with $\mathrm{AGG}(\cdot)$ and σ as the aggregation and activation functions, respectively. After L layers, h_i undergoes a projection for final prediction.

2.2 Mechanistic Models

Empirical models [37, 38] in epidemic forecasting utilize historical data to discern patterns and forecast the future spread of diseases. In contrast, mechanistic models [39, 40] provide a detailed framework that explores the biological and social complexities underlying the transmission of infectious diseases, thus exceeding the reliance on historical data inherent to empirical models. Among mechanistic approaches, classic compartmental models [41] (*e.g.*, SIR) are particularly notable. These models adeptly simplify the intricate dynamics of disease transmission into digestible components. This simplification facilitates a clearer understanding of infection spread, serving as a valuable tool for both researchers and policymakers.

SIR Compartmental Model. In the domain of epidemiology [42, 43], it is widely hypothesized that the rate at which networks evolve is significantly slower compared to the propagation speed of diseases. This fundamental assumption underpins the adoption of a SIR model [41, 44], which is instrumental in accurately capturing the dynamics of epidemic spread. The SIR model categorizes the population into three distinct groups based on their disease status: susceptible (S) to infection, currently infectious (I), and recovered (R), with the latter group being immune to both contraction and transmission of the disease. The SIR model, formulated using ordinary differential equations (ODEs) [45], are as follows:

$$\begin{gathered}\frac{dS(t)}{dt} = -\beta\frac{S(t)I(t)}{N}, \quad \frac{dI(t)}{dt} = \beta\frac{S(t)I(t)}{N} - \gamma I(t), \\ \frac{dR(t)}{dt} = \gamma I(t).\end{gathered} \tag{3}$$

These equations distribute the total population N across the aforementioned categories, with the transitions between states regulated by two pivotal parameters: the transmission rate β ($S \to I$) and

Table 1: A brief description of epidemic tasks we categorized.

Tasks	Time Interval	Objective
Detection	History-Present	Incident Back-tracing
Surveillance	Present	Event Monitoring
Prediction	Future	Future Incident Prediction
Projection	Future	Change Simulation and Prediction

the recovery rate γ ($I \longrightarrow R$). The model posits a quadratic relationship for disease transmission via interactions between susceptible and infectious individuals ($\beta S(t)I(t)$), alongside a linear recovery mechanism ($\gamma I(t)$). By fine-tuning the parameters of the SIR model, it is possible to compute the basic reproduction number $R_0 = \beta/\gamma$, serving as a metric for the disease transmission potentials [46, 47].

SIR Variants. The SIR model's simplicity overlooks factors like incubation periods and non-permanent immunity, prompting the development of more detailed SIR variants. These include: **i)** SEIR [48]: Adds an 'Exposed' compartment for those exposed but not yet infectious [41, 49], enriching the SIR model to better capture disease progression stages: $S \longrightarrow E \longrightarrow I \longrightarrow R$. **ii)** SIRD: Introduces a 'Dead' compartment to account for disease mortality, altering the progression to: $S \longrightarrow I \longrightarrow R \longrightarrow D$. This modification accounts for individuals who succumb to the disease [50, 51, 52].

The EpiLearn Library. To facilitate the development of mechanistic models and promote their integration with neural models, a Python library named **EpiLearn** [53] has recently been developed for the benefit of both epidemiologists and data scientists. It provides a comprehensive set of tools for simulating data, training and evaluating epidemic models, as well as visualizing epidemic data. For more details, we recommend referring to the paper.

3 Taxonomies

3.1 Epidemiological Tasks

For epidemiological tasks, we provide a taxonomy from the perspective of epidemiologists and categorize the work into four categories based on researchers' goals: **Detection**, **Surveillance**, **Prediction**, and **Projection**. A brief comparison of these tasks is shown in Table 1; the detailed explanations are introduced as follows:

3.1.1 *Detection.*

The goal of detection tasks is to identify health states, disease spread, or other related incidents that happened at a specific time. In this survey, we incorporate two different detection tasks from the view of graph data: *source detection* and *transmission detection.* To formulate a mathematical definition, the temporal network, which consists of sequenced graphs from different time points, is represented as $G = \{G_0, G_1, \ldots, G_T\}$. Within a graph G_t, the states of nodes and edges are represented by S_t^V and $S_t^{\mathcal{E}}$ respectively. Then, the detection task can be expressed as predicting S_t^V or $S_t^{\mathcal{E}}$ given graph G_T and time point t.

For example, finding patient-zero [74, 54, 47], as a source detection task, is important for identifying the source of disease outbreaks and aims to find a set of nodes V on graph G_0. In this setting, the problem can also be seen as identifying the state of each node at the initial time point, which is S_0^V.

3.1.2 *Surveillance.*

Surveillance tasks aim at providing timely and accurate information to support decision-making and disease prevention. Since a prompt response is needed, real-time processing ability has been the most important requirement during modeling. Here, we provide a formal definition: given a temporal graph $G = \{G_0, G_1, \ldots, G_T\}$, the goal is to identify a target statistic $\mathbf{y}$ on graph G_T at the present moment or in the short term.

To illustrate, tasks like detecting infected individuals promptly [75] and estimating infection risks in different locations in real-time [55, 56, 76, 46] can be seen as surveillance tasks, as they their prediction targets lie in present or near future.

3.1.3 *Prediction.*

Similar to surveillance tasks, prediction tasks also aim to forecast epidemic events using historical data. However, unlike surveillance tasks, prediction tasks typically involve longer time spans and do not require real-time processing. Therefore, prediction tasks are more interested in predicting the target at the longer time ahead like $T + 1$ instead of at time T. Due to the large amount of work, we further classify prediction tasks into two categories based on the type of prediction target:

(1) *Incidence Prediction.* The target of incidence prediction is to provide quantitative results. In epidemic forecasting, incidences can include the number of infections or deaths in the future [77, 78, 79, 80, 64, 65, 81, 82, 83], influenza activity level [84], Influenza-Like Illness (ILI) rates [85], vaccine hesitancy [86], etc. The prediction of these incidences is important to decision-making, proactive public health planning, and the effective management of infectious diseases and other health challenges.
(2) *Trend Prediction.* Different from incidence prediction tasks, the target of trend prediction tasks is to identify epidemic spreading patterns. For transmission among locations [59], prediction of infection trend is formulated as an information retrieving problem and the goal is to predict the next region to be infected given a historic spreading route. For transmission among individuals or groups, the goal usually includes identifying transmission dynamics in emerging high-risk groups [87].

3.1.4 *Projection.*

Projection tasks are similar to prediction tasks, but with an additional intention to understand epidemic outcomes. These tasks usually require models with the ability to incorporate changes during the evolution of epidemics. Most of the projection tasks we collected involve finding the *optimal interventions* or *maximizing influence* to achieve targets like curbing the spread of diseases. Influence maximization [88] aims to identify a subset of nodes so that the epidemic spreads most effectively across the graph, e.g., node importance ranking [89, 90].

In this paper, we extend the traditional setting of influence maximization and combine it with intervention strategy tasks to form a more general definition as follows: Given a temporal graph $G = \{V(t), \mathcal{E}(t)\}$, the states of nodes $\in V$ and edges $\in \mathcal{E}$ are influenced by strategies defined as $P_v(t)$ and $P_{\mathcal{E}}(t)$, which represents strategies on nodes and edges respectively. The goal of the task is to find optimal strategies so that the target is maximized or minimized. For example, vaccine strategy tasks [57] aim to vaccinate the optimal set of nodes to minimize epidemic damage. For interventions throughout the period, strategies can include applying quarantine level to nodes [58] and restricting mobility on edges [91, 27], which denotes $P_v(t)$ and $P_{\mathcal{E}}(t)$.

3.1.5 *Perspectives from Data Scientists.*

Besides the epidemiologists' perspective, it is also feasible to categorize these works from

Table 2: Summary of epidemiological tasks and representative GNN-based methods.

Task	Paper	Methodology	Hybrid	Graph Construction
Detection	SD-STGCN [54]	GAT + GRU + SEIR	✓	Spatial-Temporal Graph; Static Graph Structure
Surveillance	WDCIP [55]	GAE		Spatial Graph; Static Graph Structure
	GraphDNA [56]	GCN + LSTM		Spatial-Temporal Graph; Dynamic Graph Structure
Projection	MMCA-GNNA [57]	GNN + SIR + RL	✓	Spatial-Temporal Graph; Static Graph Structure
	DURLECA [27]	GNN + RL		
	IDRLECA [58]	GNN + RL		Spatial-Temporal Graph; Dynamic Graph Structure
Prediction	DGDI [59]	GCN + Self-Attention		Spatial Graph; Static Graph Structure
	DVGSN [60]	GNN		Temporal-Only Graph; Static Graph Structure
	STAN [22]	GAT + GRU		Spatial-Temporal Graph; Static Graph Structure
	MSDNet [61]	GAT + GRU + SIS	✓	
	SMPNN [62]	MPNN + Autoregression		
	ATMGNN [63]	MPNN/MGNN + LSTM/Transformer		
	DASTGN [64]	GNN + Attention + GRU		
	MSGNN [65]	GCN + N-Beats		
	STEP [66]	GCN + Attention + GRU		
	GSRNN [67]	GNN + RNN		
	Mepo GNN [68, 23]	(TCN + GCN) + Modified SIR	✓	Spatial-Temporal Graph; Dynamic Graph Structure
	Epi-Cola-GNN [25]	Cola-GNN + Modified SIR	✓	
	CausalGNN [21]	GNN + SIRD	✓	
	ATGCN [69]	GNN + LSTM		
	HierST [70]	GNN + LSTM		
	RESEAT [71]	GNN + Self-Attention		
	SAIFlu-Net [72]	GNN + LSTM		
	Epi-GNN [73]	GCN + Attention + RNN		
	Cola-GNN [20]	GCN + Attention + RNN		

data scientists' view. Here we provide a further taxonomy of the computational pipeline in terms of model **inputs** and **outputs**:

(1) For model inputs, they consist mainly of two elements: node features and the graph structure. Based on the temporal characteristics of nodes, we can further categorize these work into **spatial-only** tasks, **temporal-only** [85], and **spatial-temporal** tasks. In addition, based on the temporality and learnability of graph structure, we can also use **static** or **dynamic** classifications to distinguish these works.

(2) In terms of model outputs, we summarize these works as follows: **scalar**, **graph**, and **action sequence**. Scalar outputs are usually used in prediction tasks which provide indicators of the epidemic like infected cases. Some works focus on epidemic graph construction and their outputs are graphs [92, 55]. Finally, the projection tasks we collected adopt Reinforcement Learning (RL), which outputs the actions taken at each time step, forming a consecutive action sequence [57, 58, 91, 27].

3.2 Graph Construction

For graph construction, we provide a taxonomy based on the dynamicity of nodes and edges as follows.

Static Node Features. Static node features typically refer to characteristics that do not change with time. The shape of static features can be represented as $\mathbb{R}^{N\times h}$, where h refers to the number of features. Besides tasks involving time series, most GNN tasks are using static features. For example, in a contact graph in which individuals are modeled as nodes and contact information represents edges, personal characteristics like gender and age can be used as static features during training and prediction [75]. However, tasks involving time series can also use static features as additional information.

Dynamic Node Features. Contrary to static features, dynamic features represent characteristics that change through time. This type of data is commonly seen in time-series forecasting tasks and the models usually require inputs at each time point. Therefore, the shape of the dynamic features can be represented as $\mathbb{R}^{N\times T\times h}$, where T refers to the number of time points given. As an example, the number of daily confirmed cases in a region can be seen as dynamic features [73]. Although most models take in a single slice of dynamic features at each time point, some models use the entire dynamic features across time T in a single input [74].

Static Graph Structure. Static graph structures are generated from existing data, which are consistent across training or different times. For example, geographical adjacency A often links various regions (nodes) in the graph G for multi-regional tasks, using region distance or other criteria for edge weights [93, 78]. Another strategy explores human mobility or transitions, *e.g.*, linking nodes through nearest neighbors in the case of COVID-19 transmission. This method takes into consideration the distribution of the population and individual movements between various locations [59, 55]. When nodes represent individuals, contact information may be used as connections to identify disease-spreading risks [94, 95].

Dynamic Graph Structure. Determining the structure of a dynamic graph commonly involves one of two methodologies. One approach is the modification of adjacency relations over time or throughout the virus propagation process. For example, [91] utilize $\mathcal{E}(t) = \{e_{uv}(t)\}$ to represent the set of edges at time step t, which

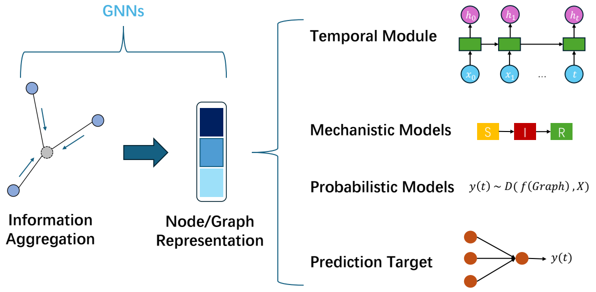

Figure 1: GNNs aggregate information from neighborhoods.

connect individuals based on transmission probability. Another strategy entails the learning of adaptive edges or edge weights during the training phase. Given the dynamic nature of disease transmission, which evolves at each time step, traditional geographical adjacency matrices fall short of accurately representing true connectivity. Recent studies [51, 20, 23] have aimed for models to learn an adaptive relationship between nodes. This typically involves initially generating node features via a neural network, followed by the computation of an attention matrix to depict dynamic connectivity, often expressed as $\mathbf{A}_t = a_{i,j} \in \mathbb{R}^{N \times N}$, where $a_{i,j}$ indicates the influence of node v_j on node v_i.

3.3 Methodological Distinctions

The methodologies of the GNNs in epidemic modeling can be broadly classified into two categories: **Neural Models** and **Hybrid Models**. This classification illuminates the extent of methods that combine computational techniques with epidemiological insights. Both categories employ neural networks, yet they diverge in their underlying principles. (a) Neural Models primarily focus on a data-driven approach and leverage the power of deep learning (i.e., GNNs in our paper) to uncover complex patterns in disease dynamics without explicit encoding of the underlying epidemiological processes. (b) On the other hand, Hybrid Models represent a synergistic fusion of mechanistic epidemiological models with neural networks. This integration allows for the structured, theory-informed insights of mechanistic models to complement the flexible, data-driven nature of GNNs, aiming to deliver predictions that are interpretable, accurate, and grounded in theoretical knowledge.

4 Methodology

In this section, we provide a detailed illustration of the methods in epidemic modeling, all of which utilize GNNs as the backbone model as shown in Figure 1. We organize these approaches into two main categories, as previously introduced in Section 3.3: *Neural Models* and *Hybrid Models*. This categorization hinges on whether mechanistic models are integrated.

4.1 Neural Models

When utilizing GNNs for epidemic modeling, numerous studies have exclusively employed GNNs without incorporating mechanistic models into their tasks, which we term Neural Models. These models excel at learning from raw data, identifying complex patterns across varied inputs, and significantly boosting task performance. In this subsection, we delve into the (GNN-based) Neural Models in epidemic modeling, dissected through three perspectives: (a) **Spatial Dynamics Modeling**, (b) **Temporal Dynamics Modeling**, and (c) **Intervention Modeling**. This categorization is designed to specifically tackle the challenges of modeling the spatial spread, temporal evolution, and the impact of intervention strategies through the advanced capabilities of GNNs.

4.1.1 *Spatial Dynamics Modeling.*

One advantage of GNNs, e.g., GCN or GAT, is their ability to capture spatial relationships through various aggregation processes, which can analyze and capture the spatial dimensions of disease propagation. Numerous studies represent the inherent structure of geographical data as graph data, denoted as $\mathbf{A}$, where nodes depict regions (e.g., cities, neighborhoods, or countries), and edges describe connections between these regions (e.g., roads, flights, or potential vectors for disease transmission). Subsequently, GNNs are applied to the graph data to uncover complex relationships and dependencies at the regional level, facilitating predictions regarding disease spread across different areas [96, 97, 63, 94, 98].

In the context of GNN modeling, the significance of edge weights is paramount, as they encapsulate the intensity and nature of interactions. Within epidemiological studies, these weights are often derived from the mobility or social connectedness between regions [62, 99]. For instance, studies such as [27, 68] utilize Origin-Destination (OD) flows to quantify inter-regional mobility, thereby dynamically capturing the intensity of transmission. To further enhance the spatial context of each node within the graph, some research advocates for the implementation of positional encoding techniques [100, 101]. These techniques are designed to augment the nodes' spatial awareness. For example, *Liu et al.* [59] introduced a unique encoding for each location, denoted as $PE(k)$, with even and odd elements represented by $\sin(k/10000^{i/L})$ and $\cos(k/10000^{i-1/L})$ respectively, where L denotes the dimension of the encoding.

While GNNs have shown success in modeling spatial relations, challenges arise when dealing with varying input data. Specifically, the absence of direct structural information and the introduction of more complex structural information pose additional difficulties during modeling. To tackle these challenges, several studies have attempted solutions, as outlined below.

Adaptive Structure Learning. There are occasions when adjacency relationship information is not available in the real world, often due to data scarcity. To overcome this challenge, several studies highlight the importance of learning an adaptive structure throughout the training process [70, 69]. For instance, *Wang et al.* [69] introduced a graph structure learning module, denoted as f_θ. This module is designed to calculate node similarities, thereby representing spatial relationships as follows:

$$\begin{gathered} \mathbf{M}_1 = \tanh(f_{\theta_1}(\alpha \mathbf{X}_1)), \quad \mathbf{M}_2 = \tanh(f_{\theta_2}(\alpha \mathbf{X}_2)), \\ \mathbf{A} = \mathrm{ReLU}(\tanh(\alpha(\mathbf{M}_2 \mathbf{M}_2^\top - \mathbf{M}_1 \mathbf{M}_1^\top))), \end{gathered} \tag{4}$$

where $\mathbf{X}_1$ and $\mathbf{X}_2$ are randomly initialized, learnable node embeddings, while α represents a hyper-parameter. *Shan et al.* [92] employed a method to estimate the graph Laplacian from COVID-19 data through convex optimization of derived eigenvectors. This approach aims to identify dynamic patterns of pandemic spread among countries by analyzing their structural relationships. Additionally, inspired by recent advancements in attention-based mechanisms [102, 103, 104], a considerable portion of research suggests the use of an attention matrix to illustrate the relationships between nodes [20, 51, 105]. Notably, Cola-GNN [20] pioneers the application of additive attention in learning the adaptive structure, which is defined as follows: $a_{i,j} = \mathbf{v}^T g(\mathbf{W}^s \mathbf{h}_i + \mathbf{W}^t \mathbf{h}_j + \mathbf{b}^s) + b^v$, where g is an activation function, $\mathbf{W}^s, \mathbf{W}^t \in \mathbb{R}^{d \times D}$, $\mathbf{b}^s \in \mathbb{R}^d$, and $b^v \in \mathbb{R}$ are trainable parameters, with d as a hyperparameter controlling the dimensions of these parameters. $a_{i,j}$ reflects the impact of location j on location i. This approach allows for dynamic adaptation to changes in graph structure, effectively capturing asymmetric and complex viral transmission patterns.

Multi-Scale Modeling. Previous approaches typically operate at a singular level, overlooking the multifaceted nature of real-world epidemiological data, which encompasses multiple scales such as country, state, and community levels. For epidemiological tasks, multi-scale modeling is imperative for capturing the dynamics of disease spread across these varied levels, from individual behaviors to global dissemination. HierST [70] leverages multi-scale modeling to effectively capture the spread of COVID-19 across different administrative levels by constructing a unified graph, which encapsulates the spatial correlation dynamics both within and between these levels. To further address both local interactions and long-range dependencies, MSGNN [65] is designed to integrate influences from both immediate and broader regions on disease transmission.

4.1.2 *Temporal Dynamics Modeling.*

The temporal dynamics in epidemiological models are pivotal for capturing the evolution of disease spread. These models typically conceptualize graphs as spatio-temporal networks, underscoring the significance of temporal data in comprehending disease dynamics, and forecasting future trends [60, 106]. A particular strand of research utilizes RNN-based models (*e.g.*, LSTM or GRU), as mechanisms to extract node features. These features are then incorporated into the graph convolution process [107, 70]. A simple way [108] to achieve this by executing the concat operator: $\mathbf{h} = \text{MLP}(\mathbf{x}_t | \mathbf{x}_{t-1} | ... | \mathbf{x}_{t-d})$ where $\mathbf{h}$ is simply the output of an MLP (Multilayer Perceptron) over the node features $\mathbf{x}$ at time t reaching back d days. Another surge of approaches executes graph spatial convolution in each time step separately, and then leverages all outputs of the GNNs as the input of the temporal module and utilizes them for final downstream tasks like the prediction [22, 106, 109, 110]. STEP [66] execute the multi-layers graph convolution operation to get all node embedding $\mathbf{h}$, and then leverage the GRU to get the final output: $\mathbf{h}_t = \mathbf{z}_t \circ \mathbf{h}_{t-1} + (1 - \mathbf{z}_t) \circ \mathbf{h}'_t$, where $\mathbf{h}_t$ is the final result, and $\mathbf{z}_t$ is the result of the update gate, which controls the inflow of information in the form of gating. The Hadamard product of $\mathbf{z}_t$ and $\mathbf{h}_{t-1}$ represents the information retained to the final memory at the previous timestep.

In contrast to the initial two methodologies, numerous studies achieve their final output by iteratively layering GNN and temporal models [111]. Some work [112, 54] advocate for the employment of Spatio-Temporal Graph Neural Networks (STGNNs) [113, 114, 115] to extract insights from multivariate spatiotemporal epidemic graphs. An STGNN integrates many ST-Conv blocks, which comprise a spatial layer flanked by two temporal layers. Each temporal layer features a 1-D CNN operating along the time axis, followed by a Gated Linear Unit (GLU), to delineate the temporal dynamics. The spatial layer utyeahilizes a GCN based on the Chebyshev polynomials approximation [116, 117] for spatial analysis. To further refine the understanding of spatial dynamics during disease evolution, RESEAT [71] proposes the continuous maintenance and adaptive updating of an attention matrix. This process aims to capture regional correlations throughout the input data period:

$$tp^t_{i,j}(\mathbf{A}) = \mathbf{A}^t_i \cdot \mathbf{A}^t_j, \quad \mathbf{A}^{t+1}_{i,j} = \text{softmax}(a^{t+1}_{i,j} + tp^t_{i,j}(\mathbf{A})),$$

where $\mathbf{A}^t_{i,j} \in \mathbb{R}$ denotes the attention weight between regions i and j at time step t; then $Att_i = \sum_{j=1}^{N} \mathbf{A}^t_{i,j} \cdot \mathbf{x}_j$ is employed as the final feature for the node v_i. Through this mechanism, RESEAT adeptly captures not only temporal patterns but also the dynamically evolving regional interrelationships. To integrate explicit observations with implicit factors over time, *Cui et al.* [105] introduced a new case prediction methodology within an encoder-decoder framework. They contend that relying solely on observed case data, which can be inaccurate, may impair prediction performance. Accordingly, their proposed decoder is designed to incorporate inputs of new cases and deaths, thereby dynamically reflecting temporal changes.

4.1.3 *Intervention Modeling.*

Intervention modeling offers a detailed perspective on epidemic spread by simulating the behaviors and interactions of individuals within a network based on intervention strategies. This method provides an intricate view of individual actions, mobility patterns, and the likelihood of disease transmission. When combined with GNN, this approach enhances the model's capability to represent the diversity and complexity inherent in real-world social networks. *Song et al.* [27] introduced a reinforcement learning framework that dynamically optimizes public health interventions to strike a balance between controlling the epidemic and minimizing economic impact. To delve deeper into the individual underlying dynamics, *Meirom et al.* [91] proposed a dual GNN module strategy. One module updates the node representations according to dynamic processes, while the other manages the propagation of long-range information. Subsequently, they employ RL to modulate the dynamics of social interaction graphs and perform intervention actions on them.

IDRLECA [24] embodies a novel integration, combining an infection probability model with an innovative GNN design. The infection probability model calculates the current likelihood of each individual's infection status. This information, along with personal health and movement data, is utilized to forecast virus transmission through human contacts using the GNN:

$$p_{i,\text{infected}} = 1 - \hat{p}_{i,\text{healthy}} = 1 - p_{i,\text{healthy},T} \times (1 - p_c)^{\text{contacts}}, \tag{5}$$

here $p_{i,\text{infected}}$ represents the probability that individual i is infected, while $p_{i,\text{healthy},T}$ denotes the baseline probability of individual i being healthy at time T, before accounting for contact-related risks. p_c refers to the probability of infection from a single contact. Additionally, a custom reward function is designed to simultaneously minimize the spread of infections and the associated costs, striking a balance between health objectives and economic considerations:

$$r = -\left(\exp\left(\Delta I/\theta_I\right) + \exp\left(\Delta Q/\theta_Q\right)\right). \tag{6}$$

This function considers the change in the number of infections (ΔI) and the cost of mobility interventions (ΔQ), with θ_I and θ_Q acting as soft thresholds for these changes.

4.2 Hybrid Models

Unlike Neural Models described above, Hybrid models merge neural networks' predictive power with mechanistic models' fundamental principles, boosting accuracy and interpretability. These can be split into *Parameter Estimation for Mechanistic Model* and *Mechanistic Informed Neural Model*. The former updates mechanistic model parameters with neural networks to reflect current epidemic trends, while the latter integrates mechanistic priors into neural networks, infusing domain knowledge and guiding learning toward realistic disease dynamics. This approach leverages neural models' data-driven insights while grounding predictions in epidemiological theory for a well-rounded epidemic prediction strategy.

4.2.1 Parameter Estimation for Mechanistic Models. This line of research highlights that hybrid models, which integrate neural networks, dynamically adjust the parameters of mechanistic models. This combination enables the analysis of real-time data, thus informing and refining mechanistic models to ensure their simulations accurately mirror the dynamics of actual epidemics [57, 61, 98]. Notably, studies like [98, 118] employ GNNs to estimate the contact (transmission) rate, β, and to monitor the epidemic evolution through the implementation of the SIR model. Further, research [22, 61] estimates both the transmission rates β and recovery rates γ by leveraging outputs from the GNN. This methodology initiates with the utilization of GRU to derive node embeddings $\mathbf{h}$, which subsequently facilitate the calculation of parameters:

$$\beta, \gamma = \mathrm{MLP}_1(\mathbf{h}) \qquad \Delta I, \Delta R = \mathrm{MLP}_2(\mathbf{h}), \tag{7}$$

where ΔI and ΔR denote the daily increases in the number of infected and recovered cases, respectively. To enhance the model's ability to leverage the dynamics of the pandemic for regulating longer-term progressions, the researchers utilize the predicted transmission and recovery rates to calculate predictions based on the dynamics of the disease spread:

$$\begin{aligned} \hat{\Delta I}^d &= \left[\hat{\Delta I}^d_{t+1}, \hat{\Delta I}^d_{t+2}, ..., \hat{\Delta I}^d_{t+L_p}\right], \\ \text{each } \hat{\Delta I}^d_i &= \beta S_{i-1} - \gamma I_{i-1} = \beta(N_p - \hat{I}^d_{i-1} - \hat{R}^d_{i-1}) - \gamma \hat{I}^d_{i-1}, \\ \hat{\Delta R}^d &= \left[\hat{\Delta R}^d_{t+1}, \hat{\Delta R}^d_{t+2}, ..., \hat{\Delta R}^d_{t+L_p}\right], \text{ each } \hat{\Delta R}^d_i = \gamma I^d_{i-1}, \end{aligned} \tag{8}$$

where I^d_{i-1} and R^d_{i-1} are calculated using the previous day actual infected and recovered cases. N_p is the population size, t time steps, and L_p is the forecast horizon. The researchers then propose two loss functions for short and long-term pandemic trends.

To go beyond single-region recognition, MepoGNN [68, 119] extends the SIR model to the metapopulation variant [120, 121, 122], accommodating heterogeneity within populations and incorporating human mobility to model the spread between sub-populations:

$$\begin{aligned} \frac{dS_i(t)}{dt} &= -\beta_i(t) \cdot S_i(t) \sum_{j=1}^{N} \left(\frac{h_{ji}(t)}{P_j} + \frac{h_{ij}(t)}{P_i}\right) I_j(t), \\ \frac{dI_i(t)}{dt} &= \beta_i(t) \cdot S_i(t) \sum_{j=1}^{N} \left(\frac{h_{ji}(t)}{P_j} + \frac{h_{ij}(t)}{P_i}\right) I_j(t) - \gamma_i(t) \cdot I_i(t), \\ \frac{dR_i(t)}{dt} &= \gamma_i(t) \cdot I_i(t). \end{aligned} \tag{9}$$

MepoGNN incorporates a spatio-temporal GNN designed to learn three dynamic parameters: $\beta_i(t+1)$, $\gamma_i(t+1)$, and $\mathbf{H}(t)$, throughout the evolving timeframe. Here, $\mathbf{H}(t)$ signifies the epidemic propagation matrix, capturing human mobility between regions, represented by $\{h(t)_{ij} | i, j \in \{1, 2, ..., N\}\}$. The model thereby generates its final prediction of daily confirmed cases as follows:

$$y_i(t) = \beta_i(t) \sum\nolimits_{j=1}^{N} \left(h_{ji}(t)/P_j + h_{ij}(t)/P_i\right) I_j(t), \tag{10}$$

Recent work [25] integrates the Cola-GNN [20] framework with the SIR model through the development of Epi-Cola-GNN, introducing a mobility matrix Π to capture the dynamics of infectious disease spread across different locations. Within this matrix, π_{ij} quantifies the intensity of human mobility from location i to location j, offering a nuanced perspective on the spatial transmission of diseases. This incorporation leads to a modification in the representation of infectious cases within the SIR model framework:

$$\frac{dI_i}{dt} = \beta_i I_i - \gamma_i I_i - \sum_{j=1, j \neq i}^{N} \pi_{i,j} I_i + \sum_{j=1, j \neq i}^{N} \pi_{j,i} I_j. \tag{11}$$

Furthermore, they introduce the concept of the Next-Generation Matrix (NGM) [123], which provides a clearer epidemiological interpretation and more effectively supports both intra-location spread and inter-location transmission influenced by human mobility.

Instead of simply estimating the rates, EpiGCN [124] innovates by using three separate linear layers to convert node features into SIR states, improving the model data awareness:

$$S_v = \sigma(\mathbf{W}_s \cdot \mathbf{h}_v + b_s), I_v = \sigma(\mathbf{W}_i \cdot \mathbf{h}_v + b_i), R_v = \sigma(\mathbf{W}_r \cdot \mathbf{h}_v + b_r).$$

Subsequently, they refine the process of updating the SIR model (Eq. (3)) and introduce a novel SIR message-passing mechanism that aggregates information from neighboring nodes. This approach modifies the conventional SIR update equation to incorporate spatial dependencies and interactions within the network:

$$\begin{gathered} S_v = S_v - \mathbf{W}_{\text{tran}} \cdot \text{concat}\left(S_v, \sum\nolimits_{\mathbf{w} \in \mathbf{A}_v} e_w I_w\right), \quad R_v = R_v + \mathbf{W}_{\text{recov}} \cdot I_v, \\ I_v = I_v + \mathbf{W}_{\text{tran}} \cdot \text{concat}\left(S_v, \sum\nolimits_{\mathbf{w} \in \mathbf{A}_v} e_w I_w\right) - \mathbf{W}_{\text{recov}} I_v, \end{gathered}$$

where $\mathbf{W}_{\text{tran}} \in \mathbb{R}^{2D \times D}$ and $\mathbf{W}_{\text{recov}} \in \mathbb{R}^{D \times D}$ denote the matrices for linear transformations corresponding to the transmission and recovery processes, respectively. Ultimately, the SIR states are concatenated and transformed to align with the prediction objectives:

$$y_v = \text{softmax}\left(\mathbf{W}_{\text{output}} \cdot \text{concat}(S_v, I_v, R_v)\right). \tag{12}$$

4.2.2 Mechanistic-Informed Neural Models. Unlike previous methods wherein neural networks dynamically adjust the parameters of mechanistic models based on data inputs, *mechanistic-informed neural models* utilize domain knowledge from mechanistic models to inform the architecture and learning processes of GNNs. This strategy flexibility allows for a swift adaptation to changing conditions, markedly improving the accuracy of forecasts and the effectiveness of interventions. Certain studies [125, 55, 95] utilize the SIR model to generate target data by simulating epidemic spreads from individual nodes, which are then employed to train GNNs for downstream tasks. In the context of source detection tasks, such as those discussed in [26, 47, 54], one-hot encoded node states $x_i^t \in \{0, 1\}^M$, with M representing the number of possible states, are used as inputs for the GNN, where the states are defined as either {S, E, I, R} or {S, I, R}. *Song et al.* [27] integrated SIHR (a variant of SIR) [126] simulation environment with the RL framework, providing a dynamic model of epidemic progression for the RL agent. This capability allows the agent to account for individuals who are hospitalized, enabling the dynamic modification of mobility control policies.

To explicitly capture causal dynamics, CausalGNN [21] introduces a novel approach to causal modeling by leveraging causal features $\mathbf{Q}_t = (q_{i,t}) \in \mathbb{R}^{N\times 4}$, with $q_{i,t} : S_i(t), I_i(t), R_i(t), D_i(t)$ representing the cumulative number of individuals in each state of the SIRD model. A causal encoder is then designed to transform these causal features into node embeddings, operating as follows:

$$\mathbf{H}_c^t = \tanh(\mathbf{Q}_t \mathbf{W}_e^t + b_e^t) \in \mathbb{R}^{N\times D}, \tag{13}$$

where $\mathbf{W}_e^t \in \mathbb{R}^{4\times D}$ and $b_e^t \in \mathbb{R}^D$ denote model parameters, and these causal features are intended to be concatenated with other node embeddings. The spatial GNN architecture also infers the SIRD rates $\beta_i(t), \gamma_i(t), \rho_i(t)$ by providing $\mathbf{P}_t = (p_{i,t}) \in \mathbb{R}^{N\times 3}$, which are subsequently utilized for SIRD model updates.

5 Future Work

While many challenges have been addressed in the application of GNNs within epidemic modeling, this field continues to confront various difficulties unexplored. This section will discuss these issues and suggest directions for future research.

Epidemic at Scales. Multi-scale data are crucial in epidemiology as they offer comprehensive insights into both intra-region and inter-region relationships . Presently, several studies have acknowledged this importance and initiated the integration of multi-scale data into their frameworks [83, 127, 128, 70]. Although these efforts have yielded models capable of accommodating multi-scale data, existing approaches are limited to processing only two predefined scales, such as county-level and state-level data. Thus, there is growing anticipation for the development of novel models capable of incorporating data across multiple dynamic scales and adaptable to diverse epidemiological tasks. Meanwhile, scalability must also be considered for numerous reasons: (1) A smaller granularity results in the expansion of graph data. (2) Some tasks require real-time processing [127]. While the number of countries or provinces can be small, the graph for individuals or other necessary parts in epidemic models can be extremely large, e.g., contact information graphs in metropolises, which could make the current methods very time-consuming. Moreover, the use of multi-scale data and the demands for real-time processing make the problem even harder.

Cross-Modality in Epidemiology. The integration of multi-modal data in epidemiological tasks offers a powerful approach for learning disease transmission dynamics, improving predictive accuracy, enabling early intervention, and fostering interdisciplinary collaboration to address public health challenges more effectively. Data from different modalities can not only serve as augmentations for each other but also compensate for noise from single-modality data. In recent years, some works have successfully incorporated multi-modality in GNNs. Although GNNs are very suitable for information aggregation and handling multi-modality data, there has not been much work exploring the multi-modality of GNNs in an epidemiology setting. Some related works [129, 46] have utilized unstructured data like textual or image data to construct node features. However, there is no cross-modality in terms of node features.

Epidemic Diffusion Process. The diffusion process, the key component in epidemiological tasks, can be both spatial and temporal. All GNN-based methods discussed above involve information aggregation at one or several time points in a discrete manner. However, in the real world, disease spreading is a continuous process, which is incompatible with current methods. To address this problem, Continuous GNNs [130, 131, 132], inspired by Neural ODE [133], can be applied to model the continuous spreading process. Another challenge arises from the temporal nature of disease transmission and infection processes, which can occur asynchronously. The work [64] considers different time-space effects and models the effects using the attention mechanism. Yet, it is still done in a discrete manner, creating gaps in the real-world transmission process.

Interventions for Epidemics. In epidemiology, control measures are vital for controlling disease spread and safeguarding public health. They include intervention strategies like vaccination, quarantine, and public health education to limit transmission and minimize outbreaks, ultimately saving lives and reducing the burden on healthcare systems [134, 135, 136]. Among the methods mentioned in this paper, most of the research incorporates intervention strategy in agent-based models [58, 91, 27] or other neural models [93]. Generally, the interventions in these methods include deleting nodes, altering nodes, and altering edge weights. However, each method only includes one type of intervention, either node-level or edge-level. In practice, however, interventions can happen at different graph levels and also at different scales. To better model the real situation, multi-level interventions need to be introduced.

Generating Explainable Predictions. Epidemic modeling seeks not just accurate forecasts but also interpretability, crucial for making informed decisions based on model predictions. Interpretability allows for understanding disease dynamics, identifying risk factors, and assessing uncertainty. Despite its importance, neural models have often overlooked interpretability, with hybrid models depending on mechanistic models for explanations. However, recent efforts to enhance GNN interpretability [137, 138, 139] could prove valuable in epidemiology, suggesting a growing recognition of the need for models that can explain their predictions in this critical field.

6 Conclusion

In this survey, we offer a comprehensive overview of Graph Neural Networks in epidemic modeling. First, we introduce the fundamental concepts relevant to both GNNs and epidemic modeling. Following this, we propose detailed and organized taxonomies for existing epidemiological tasks, datasets, and graph construction. In terms of methodologies, we have systematically categorized the literature into two primary groups: Neural Models and Hybrid Models, thoroughly reviewing the characteristics of current work in each category. Finally, we identify and discuss some of the persistent challenges, providing insightful directions for future research. The primary goal of this survey is to promote a more seamless integration of GNNs into epidemiology, motivating both epidemiologists and data scientists to delve into this rapidly advancing area.

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