Wasserstein Graph Neural Networks for Graphs with Missing Attributes

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ABSTRACT
Missing node attributes is a common problem in real-world graphs. Graph neural networks have been demonstrated power in graph representation learning while their performance is affected by the incompleteness of graph information. Most of them are not specified for missing-attribute graphs and fail to leverage incomplete attribute information effectively. In this paper, we propose an innovative node representation learning framework, Wasserstein Graph Neural Network (WGNN), to mitigate the problem. To make the most of limited observed attribute information and capture the uncertainty caused by missing values, we express nodes as low-dimensional distributions derived from the decomposition of the attribute matrix. Furthermore, we strengthen the expressiveness of representations by developing a novel message passing schema that aggregates distributional information from neighbors in the Wasserstein space. We test WGNN in node classification tasks under two missing-attribute cases on both synthetic and real-world datasets. In addition, we find WGNN suitable to recover missing values and adapt them to tackle matrix completion problems with graphs of users and items. Experimental results on both tasks demonstrate the superiority of our method.

KEYWORDS
Graph representation, Message passing, Missing-attribute graph, Node classification, Matrix completion.

1 INTRODUCTION
Graphs are ubiquitous data structures, where nodes usually have associated attributes. There have been many impressive and practical machine learning methods on graphs, particularly, graph representation learning [13, 15, 29] which attempts to embed local structural and attribute information into node representations. Graph representation learning methods underlay various downstream graph-based learning tasks such as node classification and link prediction while the accuracy of most applications is affected by the completeness of graph data. Unfortunately, missing attributes are common in many real-world graph data. For instance, in social networks such as Facebook and Twitter, users tend to hide or selectively publish their personal information for privacy concerns. In molecular networks like protein-protein association networks [32], where nodes represent proteins and edges indicate biological associations, it is difficult to obtain complete information about the sequences and molecular structures of newly discovered proteins. In general, we can categorize node attribute missing issues into two cases: 1). Entirely missing: missing entire attributes on some nodes, 2). Partially missing: missing partial attributes on all nodes. In this paper, we investigate graph learning on graphs with missing-attribute.

Existing graph representation learning methods are not specified for missing-attribute graphs. Random-walk based network embedding approaches [15, 29] exploit graph structure information to preserve pre-specified node similarities in the embedding space without considering informative node attributes. Message-passing [13] based graph neural networks (GNNs) incorporate node attributes and graph structure effectively by aggregating information from neighborhoods. However, to handle incomplete node attributes, they usually need to leverage matrix imputation techniques [18, 33] for missing values estimation before learning. Despite missing value imputation (MVI) being a well-studied problem in data mining and analysis, it is still a big challenge to recover missing values with inadequate observed information [9, 24]. Moreover, imputation methods might introduce noise in representations and restrict graph embedding approaches to model uncertainty caused by missing attributes.

In this paper, we propose a significant assumption on data: attributes of each node are sampled from low-dimensional mixture distributions, similar to the low-rank assumption in most matrix imputation algorithms. More precisely, we assume that there are some latent factors of nodes and each node has a distribution over these latent factors, called node-factor distribution. Meanwhile, each latent factor has a distribution over node attributes, called factor-attribute distribution. For instance, in text mining where nodes represent documents with words as their attributes, topics are their latent factors [1]. In practice, the number of (principal) latent factors is usually small. Following this assumption, we employ a matrix-factorization-based method to obtain latent factors from observed node attributes. Thereby, we can also get the node-factor distributions of each node which are exactly low-dimensional node distributional representations. In this way, we can capture the uncertainty caused by incomplete attribute information.

To handle various graph learning tasks on missing-attribute graphs, we develop an ingenious graph embedding framework, Wasserstein Graph Neural Network (WGNN), which can generate powerful node representations. Although the aforementioned node distributional representations incorporate attribute and uncertainty information, they fail to reflect graph structure information which is essential for graph learning. Inspired by message-passing based GNNs, we adapt the neighborhood aggregation process in GNNs
to the node distributional representations. The key idea is to generalize Mean(·) aggregator function to Wasserstein space [12] by computing the Wasserstein Barycenters - the mean of distribution of neighbors for node distributional representation update. In addition, we can pull node distributions back to the original Euclidean space and generate new Euclidean embeddings. Figure 1 depicts the general architecture. WGNN combines the propagation process with a multi-layer perceptron layer (MLP).

To comprehensively investigate the representation ability of WGNN, we design a SVD-based WGNN variant WGNN_svd for node classification concerning two missing-attribute cases: partially missing and entirely missing. We validate the strengths of our proposed framework on both synthetic and real-world graphs. Extensive empirical results show that compared with all baselines, WGNN_svd greatly boosts the performance. Furthermore, although our framework is not originally designed for missing values prediction, it can be naturally adapted for the matrix completion task with additional reconstruction constraints. Compared with SOTA matrix completion algorithms [17, 27, 30, 38], our method relies on much fewer parameters and has competitive performance.

Contributions. Overall, our contribution can be summarized as follows: 1. We propose a novel missing-attribute graph learning framework in Wasserstein space, called WGNN, to elegantly generate powerful node representations without explicit data imputation. Our performance is far surpassing that of baselines; 2. We extend WGNN on multi-graph and adapt it for matrix completion with the content of users and items and achieve comparable results of SOTA algorithms with much fewer parameters.

2 BACKGROUND AND RELATED WORK

Graph representation learning. In this paper, we focus on learning node representations on attributed graphs. There are many effective graph embedding approaches, such as DeepWalk [5], node2vec [15], GenVetor [10], which embed nodes into a lower-dimension Euclidean space and preserve graph structure while most of them disregard node informative attributes. The advent of graph neural networks [6, 13, 16, 21, 22, 35] fills the gap, by defining graph convolutional operations in spectral domain or aggregator functions in spatial domain. Although they achieved great success, they highly rely on the completeness and adequacy of attribute information.

Machine learning with missing data. To handle missing data, most machine learning methods rely on data imputation. There is a variety of missing value imputation (MVI) techniques such as mean-filling, KNN imputation [33], softimpute [18] with SVD, multivariate imputation [7, 34]. Also, many deep learning methods are proposed to perform the imputation tasks [14, 31, 36]. One work worth noting is Muzellec et al [28], which also uses optimal transport to solve the data missing problem. However, it only targets on imputation on general data (without structures) instead of graphs and has a very different methodology. The “imputing before learning” strategy has an important limitation: the performance of models is inherently constrained by the reconstruction ability of the used imputation methods. However, these imputation methods would not always work especially in the extreme missing cases.

Recently, some advanced models have been developed to directly handle missing data targeting at specified tasks. GRAPE [37] tackles missing data problems for label prediction and feature imputation. Unlike our work, the missing data is not originally on the graph nodes, but GRAPE represents their two tasks as graph-based problems by leveraging a created bipartite graph. Another recent work, SAT [8], models link prediction and node attribute imputation on missing-attribute graphs with shared-latent space assumption. Different from these works, our WGNN is a graph representation learning framework that focuses on learning node representations with incomplete attribute matrix as input without imputation; and it can be adapted to various downstream graph-based tasks.

3 WASSERSTEIN GRAPH NEURAL NETWORK (WGNN)

In this paper, we propose a graph embedding framework, named Wasserstein Graph Neural Network (WGNN) for missing-attribute graphs. WGNN (depicted in Figure 1) consists of three main components: distributional representation generation to encode observed attribute and uncertainty information, Wasserstein aggregation process to update node distributional representations involve graph structure in a low-dimensional Wasserstein space, and Euclidean representation generation to pull nodes back to a high-dimensional Euclidean space for downstream tasks.

3.1 Preliminary

3.1.1 Notations. For a matrix M, we write $M = (m_i)$, where $m_i$ is the $i$-th row of $M$. We denote $\mathcal{R}(M)$ as the set of rows of $M$ and $C(M)$ as the set of columns of $M$. Give a missing-attribute graph with a collection of node attributes $\{a_0, \ldots, a_{m-1}\}$, we denote observed attribute matrix $X^{\times m \times n} = (x_i)$ as its incomplete node attribute matrix, whose missing values are filled with zeros, and $x_i$ is the attribute vector/Euclidean embedding of the $i$-th node.

3.1.2 Assumption. We assume that observed values of $\{a_i\}$ come from a collection of $k$ latent factor vectors $\{v_{0}, \ldots, v_{k-1}\}$ where $k \ll n$ and each node (e.g. node $j$) may contain attributes from several latent distributions in particular proportions ($\mu_j$). Given $X^{\times m \times n}$, we assume that there exists low-rank matrices $W^{n \times k}$ and $B^{m \times k}$ such that $C(B)$ is the embedding of $k$ latent factors and $\mathcal{R}(W)$ is the weight/probability vectors of nodes affected by latent factors.

3.1.3 Wasserstein Distance and Wasserstein Barycenter.

- Wasserstein distance is an optimal transport metric which measures the distance traveled in transporting the mass in one distribution to match another. The $p$-Wasserstein distance between two distributions $\mu$ and $\nu$ over a metric space $X$ is defined as

$$W_p(\mu, \nu) = \left( \int_{X \times X} d(x, y)^p \, d\pi(x, y) \right)^{1/p}$$

where $\Pi(\mu, \nu)$ is the set of probabilistic couplings $\pi$ on $(\mu, \nu), d(x, y)$ is a ground metric on $X$. In this paper, we take $p = 2$. The Wasserstein space is a metric space that endows probability distributions with the Wasserstein distance.
**Wasserstein barycenter** of $N$ distributions $\{\mu_i\}$ over $X$ is an optimizer $\hat{\mu}$ to the problem:

$$\hat{\mu} = \arg \inf_{\mu \in \mathcal{P}(X)} \sum_{i=1}^{N} W_p(\mu, \mu_i),$$

where $\mathcal{P}(X)$ denotes the set of all probability measures on $X$. If $\mu_i$ are discrete distributions supported by $\text{supp}(\mu_i)$, support points of barycenter $\hat{\mu}$ must contain all possible combinations of $\text{supp}(\mu_i)$, i.e.:

$$\text{supp}(\hat{\mu}) = \left\{ \frac{1}{N} \sum_{i=1}^{N} x_i \middle| x_i \in \text{supp}(\mu_i) \right\}.$$  

(1)

### 3.2 Distributional representation generation

According to the proposed assumption, nodes are mixtures of latent factors and can be expressed as low-dimensional node-factor distributions. In this section, we develop an effective method with matrix decomposition (in our implementation, we use SVD) on the observed attribute matrix to construct a collection of principal latent factors. Thereby, we obtain latent factor embeddings and low-dimensional distributional representations $\{(\tilde{u}_i)\}$. The low-rank assumption, which is prevalent in matrix completion, allows missing value imputation methods to obtain a dense and low-rank matrix through dimension reduction techniques. In light of this, we employ SVD to the incomplete attribute matrix $X$ (similar to LSI[11]). Precisely, through compact SVD, we have $X = U\Lambda V^T$, where $U$ is so-called the principal component matrix, $\Lambda$ is a square diagonal matrix with $\Lambda_{ii} = \lambda_i$ ($\lambda_i$ are singular values of $X$ in descending order) and $V$ is the basis matrix. Here, we indicate that $C(V)$ is a collection of $m$ latent factors. For given $k \ll \min\{n, m\}$, considering the first $k$ principal latent factors, we denote $U_k = (u_i)$, $V_k = (v_i)$ and write

$$X \approx U_k \Lambda_k V_k^T.$$  

(2)

We say $U_k$ is the weight matrix with respect to $k$ latent factors with $C(V_k)$ as the embedding matrix. Allowing negative probability, $u_i$ can be regarded as a generalized discrete distribution supported by $C(V_k)$. Then we formulate a general transformation function $\phi(\cdot)$ to embed $(u_i)$ to a standard discrete probability space:

$$\hat{(u_i)} := \phi(u_i) = \frac{\phi(u_i)}{\|\phi(u_i)\|_1}. $$  

(3)

where $(\hat{(u_i)})$ is the distributional representation matrix and $\phi(\cdot)$ is a reversible non-negative function depending on data. In our implementation, $\phi(\cdot) = \exp(\cdot)$ so that $\phi(\cdot) = \text{sigmoid}(\cdot)$.

### 3.3 The Wasserstein aggregation process

Through the transformation $\phi(\cdot)$, we obtain discrete node-factor distributions $(\hat{u}_i)$ which incorporate valid observed attribute information and uncertainty of missing attributes. Noting that Euclidean embeddings fail to express the semantic information of distributions, stemming from the limited expressive capacity of Euclidean space, we take Wasserstein space as the embedding space. Similar to many graph learning methods, we attempt to reflect graph structures in node representations by aggregating information from neighbors.

We first formulate the Wasserstein distance. Denote $supp(U_k) = C(V_k)$ as the set of support points of $(\hat{u}_i)$, here we define a ground metric $d$ over $supp(U_k)$ and obtain the distance matrix $D^{k \times k}$ as...
 follows:  
\[ D_{ij} = d(C(V_k)_i, C(V_k)_j) = |\lambda_i^2 - \lambda_j^2|. \]  
(4)

Then we have the corresponding Wasserstein metric:  
\[ W_2^2(\hat{u}_i, \hat{u}_j | D) = \min_{T \geq 0} \text{tr}(DT^T) \text{ s.t. } T\mathbb{1} = \hat{u}_i, \ T^T \mathbb{1} = \hat{u}_j. \]
(5)

Recall that the mean(\cdot) aggregator function of neighborhoods in Euclidean space is  
\[ \hat{u}_i^{(l)}(\cdot) = \langle \text{mean}(\hat{u}_i^{(l-1)}, \forall j \in N(i)) \rangle, \]  
where  
\[ (\hat{u}_i^{(0)}) = (\hat{u}_i) \text{ and } N(i) \text{ is the neighborhood of node } i \text{ including } i \text{ itself.} \]
In light of this, we develop Barycenter_Update(\cdot), a generalized mean(\cdot) aggregator in Wasserstein space where we update the node distributions by aggregating the neighborhood node distributions. We indicate that Wasserstein barycenter is the mean of distributions \( \hat{u}_j^{(l)}(\cdot), \forall j \in N(i) \) in Wasserstein space. Precisely, the formulation of Wasserstein aggregation process in the l + 1-th WGN layer is:

\[ \hat{u}_i^{(l+1)}(\cdot) = \text{Barycenter_Update}(\hat{u}_i^{(l)}(\cdot), D) \]

\[ = \arg_{p \in \mathcal{P}(C(V_k))} \frac{1}{N(i)} \sum_{j \in N(i)} W_2^2(p, \hat{u}_j^{(l)} | D) \]  
(6)

where  \( \mathcal{P}(C(V_k)) \) is the set of all discrete distributions supported by  \( C(V_k) \). During the aggregation process, we fix the support of all distributions. That is, we let  \( support(\hat{u}_i^{(l+1)}(\cdot)) = C(V_k) \) with distance matrix  \( D \), for  \( i, l \). Otherwise, as the aggregation process goes on,  \( support(\hat{u}_i^{(l+1)}(\cdot)) \) will be larger and larger and cause high computation complexity (recall that  \( support(\hat{u}_i^{(l+1)}(\cdot)) \) should be \( \left\{ \sum_{j \in N(i)} x_j | x_j \in support(\hat{u}_j^{(l)}(\cdot)) \right\} \). In implementation, we use the Iterative Bregman Projection (IBP) [3] algorithm to compute such fixed-support Wasserstein barycenter (see Algorithm 1). The complexity of the Wasserstein Barycenter of  \( N \times k \)-dimensional discrete distributions by IBP is  \( O(Nk^2/e^2) \) referring to Kroshnin et al. [23]. The complexity of the Wasserstein aggregation process is  \( O(|E|k^2/e^2), |E| \) is the number of edges. In our implementation, the number of iteration  \( M = 100 \) and  \( \epsilon = 1e-2 \).

### 3.4 Euclidean representation generation

Matrix factorization separates the observed attribute information into two parts and stores it in  \( U_k \) and  \( V_k \). To take full advantage of the information in  \( V_k \), we finally pull nodes back to the Euclidean space, which has the same dimension as the original feature space. Thereby, we obtain high-dimensional Euclidean embeddings.

We first convert the updated Wasserstein embeddings  \( \hat{u}_i \) to weight matrix  \( \hat{U}_k \) with  \( \hat{U}_k^T \hat{U}_k = I_k \) (recall that the initial weight matrix is derived from the orthogonal principal-component matrix), then transform it to the Euclidean embeddings  \( \hat{U}_k \):

\[
\hat{U}_k = \text{Gram Schmidt Ortho}\left( \varphi^{-1}(\hat{u}_i) \right),
\]

\[
\hat{X} = \hat{U}_k \Lambda_k \hat{V}_k^T,
\]

where Gram Schmidt Ortho is the Gram-Schmidt orthogonalization processing to maintain the orthogonality of  \( \hat{U}_k \). In our implementation,  \( \varphi^{-1}(\cdot) = \log(\cdot) \). Interestingly, empirical results show that orthogonalizing node embeddings can efficiently alleviate the over-smoothing problem. Then we can feed  \( \hat{X} \) to arbitrary neural networks to handle various downstream tasks such as node classification. Similar to most GNNs, we equip WGN with a MLP.

**Reconstruction for matrix completion.** Obviously,  \( \hat{X} \) is not a matrix completion for  \( X \) but a new Euclidean representation matrix. However, with an additional reconstruction constrains, WGN is able to recover missing values. More details are provided in Section 4.3.

### 4 Empirical Study

In this section, we examine WGN in node classification on synthetic and real-world datasets under two missing-attribute settings to verify the advantages of low-dimensional distributional embedding and Wasserstein aggregation. In addition, we adapt WGN to matrix completion problems to illustrate the capacity of missing value prediction of our proposed framework.

#### 4.1 Node classification on synthetic data

![Figure 2: A synthetic partition graph with 3 communities whose sizes are 262, 207 and 319, respectively. 3 labels are assigned to these 788 nodes (colored with red, blue and green) while 85% nodes in a community have the same label.](image-url)

We conduct synthetic experiments in node classification to illustrate the strengths of crucial components of our proposed framework. We first create synthetic data and develop some ablation models as follows.

**4.1.1 Synthetic data.** We generate a random undirected partition graph with three communities whose probabilities of internal and external connections are 0.035 and 0.005, respectively (shown in Figure 2). We randomly assign nodes with three labels such that 85% nodes in a community have the same label.
labels have different families of distributions \(\{p_0(x)\}\) over 100 attributes, i.e., Gumbel distributions, Logistic distributions, and Laplace distributions. Node attribute values are then sampled from their distributions. \(\theta\) is the random parameter of these distributions which is different for each node; and \(\{p_0(x)\}\) are exactly the node-attribute distributions that are high-dimensional. Following our proposed assumption, we can also obtain lower-dimensional node-factor distributions by decomposing the attributes through SVD.

That is, we have both low-dimensional and high-dimensional node distributional representations of this synthetic graph.

4.1.2 Missing settings. Given a full attribute matrix \(X \in \mathbb{R}^{n \times m}\), we generate incomplete input under two missing settings:

- **Partially Missing.** For partially missing rate \(r_p \in \{0.1, \ldots, 0.9\}\), we generate a mask \(M \in \{0, 1\}^{n \times m}\) with \(p(M_{ij} = 0) = r_p\) and take \(X \odot M\) as input.

- **Entirely Missing.** For entirely missing rate \(r_e \in \{0.1, \ldots, 0.9\}\), we generate a mask vector \(m \in \{0, 1\}^n\) with \(p(m_i = 0) = r_e\) and take \(X \odot m\) as input.

**Algorithm 2** WGNNevd for node classification

**Input:** incomplete matrix \(X\) filled with zeros, \(k\).

1. Apply \(k\)-rank SVD to \(X: X = U_k A_k V_k^\top\).
2. Initialize \(u_i^{(0)}\) → \(U_k\)
3. for \(l = 1\) to \(L\) do
   a. \(u_i^{(l-1)} = \text{Gram Schmidt Ortho}(\log(u_i^{(l-1)}))\)
   b. \(u_i^{(0)} = (u_i^{(l-1)})\)
4. for \(l = 1\) to \(h\) do
   a. \(\hat{u}_i^{(l)} = (\arg \inf_{p \in P_i(C(V_k))} \sum_{j \in N(i)} W_{ij}^2(p, \hat{u}_j^{(l-1)}|D))\)
5. end for
6. \(u_i^{(l)} = (\sum \hat{u}_i^{(l)}) / L\)
7. \(X = (\sum \hat{u}_i^{(l)}) / L\)
8. Apply MLP for node classification: \(Y = \text{softmax}(\text{MLP}(\hat{X}))\)

4.1.3 Testing models.

- **WGNNevd.** In node classification tasks, we develop a variant of WGNNevd, named WGNNevd, using SVD to generates low-dimensional node distributions (see Algorithm 2). We denote \(L\) and \(h\) are the hyper-parameters of the number of WGNNevd layers and times of Wasserstein aggregation in each layer, respectively. We take the average output of each layer as the updated principal-component representations to avoid over-smoothing.

- **WGNNevd.** In order to verify the superiority of our proposed low-dimensional distributional representation generation method on missing-attribute graphs, we develop an ablation model WGNNevd which directly apply the Wasserstein aggregator on the high-dimensional distributional representations \(\{p_0(x)\}\).

- **WGNNevd.** To illustrate the effectiveness of latent factors embedded through SVD, we consider a collection of random latent factors. Precisely, we randomly generate a set of \(k\) orthogonal vectors \(\{b_i\}\) and denote \(B = (b_i)\) as the embedding matrix of random latent factors and obtain mixture weight matrix \(W\) and ‘singular matrix’ \(R\) such that \(X = WRB^\top\). Then we construct another ablation model WGNNevd by adapting our space transformation and Wasserstein aggregator to \((B, R, W)\).

- **GNNs and MLP.** We also compare WGNNevd with some standard baselines: MLP and two GNN models, i.e., GCN [20] and GraphSAGE[16].

4.1.4 Results. Experimental results shown in Figure 3 demonstrate that:

- When there are no missing attributes, both WGNNevd and WGNNevd still outperform other baselines including Euclidean graph embedding methods. It implies the power of Wasserstein embeddings.

- At low missing rates, WGNNevd has comparable performance with WGNNevd while it fails at high missing rates. It shows the superiority of our proposed low-dimensional distributional representation generation method, especially in extremely missing cases.

- WGNNevd has consistent poor performance across all missing attribute settings which shows the necessity of a proper matrix factorization (e.g. SVD) to figure out appropriate latent factors.

4.2 Node classification on real-world data

4.2.1 Experimental setup. **Datasets.** We conduct experiments on three Citation datasets: CORA, CITESEER and PUBMED (summarized in Table 1).

**Baselines.** We first compare against two structure-based methods: the Label Propagation Algorithm (LP) and GCNnofeat (take an identity matrix as input). For other graph learning methods, we apply different imputation approaches for data preprocessing, including zero-filling, mean-filling, soft-impute based on low-rank SVD [25], KNN-impute [2], and two deep learning techniques: GINN based on a generative adversarial networks [31], and MIDA based on a deep denoising autoencoder [14]. To compare with graph neural networks, we develop six baselines based on GCN: GCNzero, GCNmean, GCNsoft, GCNknn, GCNginn, GCN_mida and four working with GAT: GATzeros, GATsoft, GATginn and GATmida. Moreover, following the low-rank assumption, we develop an additional baseline GCNevd by feeding GCN with \(U_k A_k V_k^\top\) instead of \(X\).

It is worth noting that there is a difference between the experimental setting we use for testing MIDA baselines and the original one in our paper. As MIDA requires training data, we use 30% nodes whose attributes are complete for training. That is, with the same

| Table 1: Statistics of synthetic data and citation networks. |
|---------------------|----------|--------|------|----------|
| Dataset             | Node     | Edge   | Feature | Class   | Label Rate |
| Synthetic           | 788      | 4726   | 100    | 3        | 0.1        |
| Cora                | 2,708    | 5,278  | 1,433  | 7        | 0.052      |
| Citeeseer           | 3,327    | 4,552  | 3,703  | 6        | 0.036      |
| Pubmed              | 19,717   | 44,324 | 500    | 3        | 0.003      |
When observed information is adequate for missing value imputation, Wasserstein aggregator and obtain Euclidean embeddings for label computation complexity. In addition, low-dimensional representations can greatly reduce computation complexity.

**Model configurations.** For all experiments, we train models using Adam optimizer with 0.01 learning rate. We early stop the model training process with patience 100, select the best performing models based on validation set accuracy, and report the mean accuracy for 10 runs as the final results. We apply two-layer MLP with 128 hidden units for node prediction with fixed $k = 64$. The optimal $L$, $h$ and the layers of GCN and GAT differ in different missing levels. For partially missing, $L = 14$ and $h = 2, 4, 6$ when $r_p \in [0.1, 0.3]$, $r_p \in [0.4, 0.6]$, $r_p \in [0.7, 0.9]$ respectively. We use 2-layer GCN and GAT when $r_p \in [0.1, 0.6]$ and 4-layers when $r_p \in [0.7, 0.9]$. For whole missing, when $r_e \in [0.1, 0.5]$, $L = 10$, $h = 2$; when $r_e \in [0.6, 0.9]$, $L = 14$, $h = 6$. We use 2-layer GCN and GAT when $r_e \in [0.1, 0.3]$ and 4-layer when $r_e \in [0.4, 0.9]$.

**4.2.2 Experimental results.** As shown in Figure 4, WGGNN_{svd} has the best performance on all datasets across all entirely and partially missing levels. Even though MIDA leverages 30% more observed values, it does not show any superiority, especially in the entirely missing case. Compare with other baselines, WGGNN_{svd} exhibits significant advantages at high missing level and yields at least 6%, 10% and 9% higher accuracy when $r_e = 0.9$ and 5%, 8% and 5% higher accuracy when $r_p = 0.9$ over CORA, CITeSeer and PubMed, respectively. It implies that WGGNN can indeed greatly reduce information distortion by incorporating known semantic information and structure. Conversely, when $r_p \approx 0.9$, several baselines like GCN_{node} and GCN_{noseat} show lower performance than GCN_{noseat} on CORA and CITeSeer. It demonstrates that it is hard to recover missing values and prone to introduce noise when observed information is rare. When observed information is adequate for missing value imputation, such as more than 60% attributes are available, all methods except for LP and GCN_{noseat} have comparable performance at a low missing level. It indicates a possible limitation of WGGNN: for data with rare missing attributes, WGGNN is not necessary due to its added complexity. Simple baselines can already generate good results. In general, WGGNN shows consistently remarkable performance across all settings.

**4.2.3 Sensitive analysis.** The results of model tuning are shown in Figure 5(a). We only report the experimental results on CORA at 0.9 missing ratio on account of the similar performances on other datasets and missing ratios. Except for the curve of $L = 1(h = 5)$, all curves of $L$ have a clear trend of increasing as $h$ increases. Noting that each WGGNN layer aggregates information from $h$-hop neighbors, $L$ layers WGGNN model involves $L \times h$-hop neighbors. WGGNN_{svd} has the best performance with $L = 5, h = 9$. In this case, 45-hop neighbors are involved in the graph embedding process. As we know, many GNN models encounter the over-smoothing issue when they go deep. However, our method can efficiently handle over-smoothing. This is due to two strategies: incorporating the output of all WGGNN layers and orthogonalization which make nodes different. The curve of $L = 1(h = 5)$ provides the experimental illustration: $L = 1$ means that there is only once orthogonalization, the performance would decrease starting from $h = 4 + 5$.

**4.2.4 Ablation study.** To illustrate how WGGNN improves the performance, we develop four ablation models to test three main modules of WGGNN: low-dimensional distributional embedding module, Wasserstein aggregation module and Euclidean embedding module, respectively. For most ablation models, we report the experimental results on CORA under partially missing settings, shown in Figure 5(b).

### 1. Low-dimensional distributional embedding module. In our synthetic experiments, we show the necessity and advantages of low-dimensional embedding. Here, we verify it on real-world data. We design an ablation model WGGNN_{hd} which directly transforms node attributes to discrete distributions ($\tilde{x}_i^{(0)}$) without dimension reduction. Since the semantic information of each dimension of ($\tilde{x}_i^{(0)}$) is unknown, we simply define the ground distance matrix as $\tilde{D} = I - I$, where $I$ is all-ones matrix. Then we generate high-dimensional distributional representations leveraging our Wasserstein aggregator and obtain Euclidean embeddings for label prediction.

Even when $r_p = 0.1$, WGGNN_{hd} only has 0.439 accuracy on CORA. It is much lower than the worst baseline GCN_{noseat} whose accuracy is 0.6029. It is consistent with our synthetic experiment results. In addition, low-dimensional representations can greatly reduce computation complexity.
Figure 4: Average accuracy of node classification with different entirely missing (upper) and partially missing (lower) levels. At the highest missing level, WGNN_{svd} yields 8% higher accuracy in entirely missing case and 5% higher accuracy in partially missing case compared with the best baselines.

Figure 5: Sensitivity analysis on times $h$ of Wasserstein aggregation in each layer and the number of WGNN layers $L$ on Cora at $r_e = 0.9$ (left) and $r_p = 0.9$ (middle), and results of ablation models (right).

**ii. Wasserstein aggregation module.** By replacing Wasserstein aggregation process with GCN and Mean($\cdot$) aggregator to update low-dimensional Euclidean embedding $U_k$ in WNN framework, we develop ablation models GCN$_U$ and MEAN$_U$ to demonstrate the power of Wasserstein aggregation.

The architecture of GCN$_U$ is similar to GCN$_{svd}$:

$$Y = MLP(GCN(U_k)A_kV_k^{-1})$$

Here, the updated low-dimensional Euclidean embedding $GCN(U_k)$ is not orthogonal as Gram-Schmidt Orthogonalization is not differentiable. For MEAN$_U$, since there is no parameter involved in
The curve of WGGNsvd,U is similar to MEANU. It confirms the necessity of incorporating information of V̂k in node representations to improve the accuracy of label prediction.

4.3 Multi-Graph matrix completion

As we mentioned in Section 3.4, with additional reconstruction constrains, WGGN enables to reconstruct incomplete matrix. In this section, we test the reconstruction ability of WGGN on recommendation systems with the known pairwise relationship among users and items which is a typical matrix completion problem with user-graph and item-graph.

Multi-WGGN. For a rating matrix X, R(X) and C(X) are attribute vectors of users and items, respectively. Our proposed assumption on the node-graph allows us to express user-nodes as low-dimensional user-factor distributions based on their attributes. Similarly, we can also represent item-nodes as item-factor distributions. Precisely, we generate such distributional representations of users and items, i.e., (φ(u)) (supported by C(Vk)) and (φ(v)) (supported by C(Uk)), through transformation φ(·) formulated in Section 3.2. Then we conduct Wasserstein aggregation in the Wasserstein spaces of users and items for distributional representation update. It is worth noting that, we can perform these processes in parallel without interference since we utilize the fixed-support Wasserstein barycenter for update while the ground metrics of the two Wasserstein spaces defined as Equation (4) only depend on Λ.

Algorithm 3 Multi-WGGN for matrix completion

Input: incomplete matrix X filled with zeros, k. Apply k-rank SVD to X: X ≈ U_kΛ_kV_k^T.

Initialize (u_i^{(0)}) ← Uk, (v_i^{(0)}) ← Vk.

for l = 1 to L do

(u_i^{(l-1)}) ← \exp(u_i^{(l-1)}) / \exp(u_i^{(l-1)})

(v_i^{(l-1)}) ← \exp(v_i^{(l-1)}) / \exp(v_i^{(l-1)})

(u_i^{(0)}) ← (u_i^{(l-1)}), (v_i^{(0)}) ← (v_i^{(l-1)})

for t = 1 to h do

(u_i^{(l)}) = Gram_Schmidt_Ortho(\log(u_i^{(h)}))

(v_i^{(l)}) = Gram_Schmidt_Ortho(\log(v_i^{(h)}))

end for

(\hat{u}_i) = Concat(u_1^{(0)},...,u_L^{(k)})

(\hat{v}_i) = Concat(v_1^{(0)},...,v_L^{(k)})

\hat{U}_k = MLP_u(\hat{u}_i) / MLP_u(\hat{u}_i)

\hat{V}_k = MLP_v(\hat{v}_i) / MLP_v(\hat{v}_i)

Return \hat{X} = \hat{U}_kΛ_k\hat{V}_k^T

Table 2: Statistics of Flixster and MovieLens-100K.

| Dataset  | Users | Items | Ratings | Density | Rating types |
|----------|-------|-------|---------|---------|-------------|
| Flixster  | 3,000 | 3,000 | 26,173  | 0.0029  | 0.5,1,1.5,5 |
| ML-100K  | 943   | 1,682 | 100,000 | 0.0630  | 1.2,5      |

and splits provided by Monti et al [27]. More Statistics details are provided in Table 2.

Baselines. We compare our Multi-WGGN model against five advanced matrix completion methods including GRALS [30]: a graph regularized model utilizing alternating minimization methods and graph structure for completion; sRMCNN [26]: a geometric matrix completion method applying multi-graph CNNs to graphs of users and items; GC-MC [4]: a graph-based method representing matrix completion as link prediction on user-item bipartite graphs; F-EAE [17]: an inductive completion method leveraging exchangeable matrix layers; IGMC [38]: the state of the art matrix completion method using a GNN to enclosing subgraphs for prediction.

Table 3: RMSE test results on Flixster and MovieLens-100K.

|          | GRALS | sRMG | GC-MC | F-EAE | IGMC | Ours |
|----------|-------|------|-------|-------|------|------|
| Flixster | 1.245 | 0.926| 0.917 | 0.908 | 0.872| 0.883|
| ML-100K  | 0.945 | 0.929| 0.905 | 0.920 | 0.905| 0.910|

Experimental settings and results. We follow the experimental setup of Monti et al [27] and take the common metric Root Mean
Square Error (RMSE) to evaluate the accuracy of matrix completion. We use 4-layer MLP with 50 hidden units on all datasets. For Flickr, we choose \( k = 25, L = 3, h = 2 \). For Movielens-100K, we set \( k = 25, L = 7, h = 1 \). We train the model using Adam optimizer with 0.001 learning rate. We repeat the experiment 10 times and report the average RMSE. The baseline results are taken from Zhang et al. [38]. Table 3 shows the results. As we can see, our Multi-WGNN model has comparable performance as the best baseline IGMC. However, we only rely on a MLP, while IGMC needs to train both GCN and MLP. Furthermore, IGMC requires to extract the enclosing subgraph for each target edge, which is extremely computationally expensive. Therefore, although WGNN is not originally designed for missing value imputation, it shows powerful capacity of reconstruction.

5 CONCLUSION

Missing-attribute graphs are ubiquitous in the real world, while most graph learning approaches have limited ability to leverage incomplete information directly. In this work, we propose WGNN, a framework to generate node representations incorporating observed node attributes, structural information and uncertainty caused by missing values. The key is to transform nodes to a powerful embedding space - a low-dimensional Wasserstein space and develop a suitable message passing schema in such space - the Wasserstein aggregation process. Compared to extensive baselines, our framework shows a significant improvement in prediction, especially when observed information is rare. We further adapt the framework to perform matrix completion with multi-graph. Experiment results on recommendation systems illustrate our capacity to recover missing values.

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