Graph Convolutional Networks for Graphs Containing Missing Features

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ABSTRACT
Graph Convolutional Network (GCN) has experienced great success in graph analysis tasks. It works by smoothing the node features across the graph. The current GCN models overwhelmingly assume that node feature information is complete. However, real-world graph data are often incomplete and containing missing features. Traditionally, people have to estimate and fill in the unknown features based on imputation techniques and then apply GCN. However, the process of feature filling and graph learning are separated, resulting in degraded and unstable performance. This problem becomes more serious when a large number of features are missing. We propose an approach that adapts GCN to graphs containing missing features. In contrast to traditional strategy, our approach integrates the processing of missing features and graph learning within the same neural network architecture. Our idea is to represent the missing data by Gaussian Mixture Model (GMM) and calculate the expected activation of neurons in the first hidden layer of GCN, while keeping the other layers of the network unchanged. This enables us to learn the GMM parameters and network weight parameters in an end-to-end manner. Notably, our approach does not increase the computational complexity of GCN and it is consistent with GCN when the features are complete. We conduct experiments on the node label classification task and demonstrate that our approach significantly outperforms the best imputation based methods by up to 99.43%, 102.96%, 6.97%, 35.36% in four benchmark graphs when a large portion of features are missing. The performance of our approach for the case with a low level of missing features is even superior to GCN for the case with complete features.

KEYWORDS
Graph convolutional network, GCN, Missing data, Incomplete data, Graph embedding, Network representation learning

1 INTRODUCTION
Graphs are used in many branches of science as a way to represent the patterns of connections between the components of complex systems, including social analysis [23], product recommendation [99], web search [8], disease identification [4], brain function analysis [68], and many more [7].

In recent years there is a surge of interest in learning on graph data. Graph embedding [10, 17, 27, 30] aims to learn low-dimensional vector representations for nodes or edges [75]. The learned representations encode structural and semantic information transcribed from the graph and can be used directly as the features for downstream graph analysis tasks. Representative work on graph embedding include random walk and skip-gram model based methods [28, 55], matrix factorization based approaches [42, 49, 57, 61], edge reconstruction based methods [50, 70], and deep learning based algorithms [51, 76], etc.

Meanwhile, graph neural network (GNN) [59, 83, 96–98], as a type of neural network architectures that can operate on graph structure, has achieved superior performance in graph analysis and shown promise in various applications such as visual question answering [48], image captioning [90], action recognition [85], point clouds classification and segmentation [39, 63, 71, 74], text classification [18, 82, 89], named entity extraction [56], fraud detection [43], machine translation [5, 45], molecular fingerprints prediction [20], protein interface prediction [22], topic modeling [87], times series forecasting [54, 84], polypharmacy side effects prediction [100], and social recommendation [77, 78, 80, 92].

Among various kinds of GNNs, graph convolutional network (GCN) [37], a simplified version of spectral graph convolutional networks [18, 62], has attracted a large amount of attention. GCN and its subsequent variants can be interpreted as smoothing the node features in the neighborhoods guided by the graph structure, and have experienced great success in graph analysis tasks, such as node classification [29, 37, 72], graph classification [95], link prediction [94], graph similarity estimation [3], node ranking [13, 21], and community detection [16, 32, 33, 73].

The current GCN-like models assume that the node feature information is complete. However, real-world graph data are often incomplete and containing missing node features. Much of the missing features arise from the following sources. First, some features can be missing because of mechanical/electronic failures or human errors during the data collection process. Secondly, it can be prohibitively expensive or even impossible to collect the complete data due to its large size. For example, social media companies such as Twitter and Facebook have restricted the crawlers to collect the whole data. Thirdly, we cannot obtain sensitive personal information. In a social network, many users are unwilling to provide information such as address, nationality, and age to protect personal privacy. Finally, graphs are dynamic in nature, and thus newly joined nodes often have very little information. All these aspects result in graphs containing missing features.

To deal with the above problem, the traditional strategy is to estimate and fill in the unknown values before applying GCN. For

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Figure 1: The architecture of our model.

Based on the transformation, we derive the analytic solution to calculate the expected activation of neurons in the first layer of GCN.

We propose the whole network architecture for learning on graphs containing missing features. We prove that our model is consistent with GCN when the features are complete.

We perform extensive experiments and demonstrate that our approach significantly outperforms imputation based methods.

The rest of the paper is organized as follows. The next section summarizes the recent literature on GCN and methods for processing missing data. Section 3 reviews GCN. Section 4 introduces our approach. Section 5 reports experiment results. Finally, Section 6 presents our concluding remarks.

2 RELATED WORK

2.1 Graph Convolutional Networks

GNNs are deep learning models aiming at addressing graph-related tasks [59, 83, 96–98]. Among various kinds of GNNs, GCN [37], which simplifies the previous spectral graph convolutional networks [18, 62] by restricting the filters to operate in one-hop neighborhood, has attracted a large amount of attention due to its simplicity and high performance. GCN can be interpreted as smoothing the node features in the neighborhoods, and this model achieves great success in the node classification task.

There are series of works following GCN. GAT extends GCN by imposing the attention mechanism on the neighboring weight assignment [72]. AGCN learns hidden structural relations unspecified by the graph adjacency matrix and constructs a residual graph adjacency matrix [39]. TO-GCN utilizes potential information by jointly refining the network topology [86]. GCLN introduces ladder-shape architecture to increase the depth of GCN while overcoming the over-smoothing problem [31]. MixHop introduces higher-order feature aggregation, which enables us to capture mixing neighbors’ information [1]. UDA-GCN employs a dual GCN structure to facilitate knowledge adaptation between graphs [81]. Besides, some researchers use Hyperbolic space instead of Euclidean space to reduce the distortion of embeddings [11, 41].
Training GCN usually requires to save the whole graph data into memory. To solve this problem, sampling strategy [14, 29] and batch training [15] are proposed. Moreover, FastGCN reduces the complexity of GCN through successively removing nonlinearities and collapsing weight matrices between consecutive layers.

We note that all of the models mentioned above assume that the node feature information is complete.

### 2.2 Learning with Missing Data

Incomplete and missing data is common in real-world applications. Methods for handling such data can be categorized into two classes. The first class completes the missing data before using conventional machine learning algorithms. Imputation techniques are widely used for data completion, such as mean imputation [24], matrix completion via matrix factorization [38] and singular value decomposition (SVD) [46], and multiple imputation [9, 58]. Machine learning models are also employed to estimate missing values, such as $k$-NN model [6], random forest [69], autoencoder [26, 36, 52, 67], generative adversarial network (GAN) [40, 44, 93]. However, imputation methods are not always competent to handle this problem, especially when the missing rate is high [12].

The second class directly trains a model based on the missing data without any imputation, and there are a range of research along this line. Che et al. improve Gated Recurrent Unit (GRU) to address the multivariate time series missing data [12], Jiang et al. divide missing data into complete sub-data and then applied them to ensemble classifiers [34]. Pelckmans et al. modify the loss function of Support Vector Machine (SVM) to address the uncertainty issue arising from missing data [53]. Moreover, there are some research on building improved machine learning models such as logistic regression [79], kernel methods [64, 66], autoencoder and multilayer perceptron [65] on top of representing missing values with probabilistic density.

To the best of our knowledge, there is no related work on how to adapt GNNs to graphs containing missing features. Hence, we propose an approach to address this problem.

### 3 PRELIMINARIES

In this section, we briefly review GCN, which paves the way for the next discussion.

#### 3.1 Notations

Let us consider an undirected graph $G = (V, E)$, where $V = \{v_i \mid i = 1, \ldots, N\}$ is the node set, and $E \subseteq V \times V$ is the edge set. $A \in \mathbb{R}^{N \times N}$ denotes the adjacency matrix, where $A_{ij} = A_{ji}$, $A_{ij} = 0$ if $(v_i, v_j) \notin E$, and $A_{ij} > 0$ if $(v_i, v_j) \in E$. $X \in \mathbb{R}^{N \times D}$ is the node feature matrix and $D$ is the number of features. $S \subseteq \{(i, j) \mid i = 1, \ldots, N, j = 1, \ldots, D\}$ is a set for missing features: $\forall (i, j) \in S, X_{ij}$ is not known.

#### 3.2 Graph Convolutional Network

GCN-like models consist of aggregators and updaters. The aggregator gathers information guided by the graph structure, and the updater updates nodes’ hidden states according to the gathered information. Specifically, the graph convolutional layer is based on the following equation:

$$H^{(l+1)} = \sigma(\tilde{A}H^{(l)}W^{(l)})$$

where $L \in \mathbb{R}^{N \times N}$ is the aggregation matrix, $H^{(l)} = (h_1^{(l)}, \ldots, h_N^{(l)})^T \in \mathbb{R}^{N \times D^{(l)}}$ is the node representation matrix in $l$-th layer, $H^{(0)} = X$, $W^{(l)} \in \mathbb{R}^{D^{(l)} \times D^{(l+1)}}$ is the trainable weight matrix in $l$-th layer, and $\sigma(\cdot)$ is the activation function such as ReLU, LeakyReLU, and ELU.

GCN [37] adopts the re-normalized graph Laplacian $\hat{A}$ as the aggregator:

$$L = \hat{A} = \tilde{D}^{-1/2} \tilde{A} \tilde{D}^{-1/2},$$

where $\hat{A} = A + I$ and $\tilde{D} = \text{diag}(\sum_j \hat{A}_{ij}, \ldots, \sum_i \hat{A}_{ji})$. Empirically, 2-layer GCN with ReLU activation shows the best performance on node classification, defined as:

$$\text{GCN}(X, A) = \text{softmax}(L(\text{ReLU}(LXW^{(0)}))W^{(1)})$$

### 4 PROPOSED APPROACH

In this section, we propose our approach for training GCN on graphs containing missing features. We follow GMMC [65] to represent the missing data by GMM and calculate the expected activation of neurons in the first hidden layer. Although this idea is implemented in simple neural networks such as autoencoder and multilayer perceptron, it has not yet been extended to complex neural networks such as RNN, CNN, GNN, and sequence-to-sequence models. The principal difficulty lies in the fact that simply using GMM to represent the missing data will even complicate the network architecture, which hinder us from calculating the expected activation in closed form. In the following, we propose a novel way to unify the representation of missing features and calculation of the expected activation of the first layer neurons in GCN. Specifically, we skillfully represent the missing features by introducing only a small number of parameters in GMM and derive the analytic solution of the expected activation, enabling us to integrate the processing of missing features and graph learning within the same neural network architecture.

#### 4.1 Representing Node Features Using GMM

Suppose $X \in \mathbb{R}^D$ is a random variable for node features. We assume $X$ is generated from the mixture of (degenerate) Gaussians:

$$X \sim \sum_{k=1}^K \pi_k N(\mu[k], \Sigma[k])$$

where $K$ is the number of components, $\pi_k$ is the mixing parameter with the constraint that $\sum_k \pi_k = 1$, $\mu[k]$ and $\Sigma[k]$ denote the $k$-th element of mean and variance of the $k$-th Gaussian component, respectively. Further, we introduce a mean matrix $M[k] \in \mathbb{R}^{N \times D}$
and a variance matrix $S^{[k]} \in \mathbb{R}^{N \times D}$ for each component as:

$$
M^{[k]}_{ij} = \begin{cases} 
\hat{\mu}^{[k]}_j & \text{if } X_{ij} \text{ is missing;} \\
\bar{X}_{ij} & \text{otherwise}
\end{cases} 
$$

(7)

$$
S^{[k]}_{ij} = \begin{cases} 
(\sigma^{[k]}_j)^2 & \text{if } X_{ij} \text{ is missing;} \\
0 & \text{otherwise}
\end{cases}
$$

(8)

This enables us to represent each $X_{ij}$ with:

$$
X_{ij} \sim \sum_{k=1}^{K} \pi_k N(M^{[k]}_{ij}, S^{[k]}_{ij}),
$$

(9)

no matter whether $X_{ij}$ is missing or not. Thus, we skillfully transform the input of our model into fixed and unfixed $X_{ij}$ that follows mixture of Gaussian distributions. The next layer is based on calculation of the expected activation of neurons, which is discussed in the next section.

### 4.2 The Expected Activation of Neurons

Let us first identify some symbols that will be used. Suppose $x \sim F_x$ is a random variable and $F_x$ is the probability density function. We define

$$
\sigma[x] \triangleq \sigma[F_x] \triangleq \mathbb{E}[\sigma(x)],
$$

(10)

which is the expected value of $\sigma$ on $x$.

**Lemma 4.1.** Let $x \sim N(\mu, \sigma^2)$. Then:

$$
\text{ReLU}[N(\mu, \sigma^2)] = \sigma[N_{\frac{\mu}{\sigma}}],
$$

(11)

where

$$
\text{NR}(z) = \frac{1}{\sqrt{2\pi}} \exp \left( -\frac{z^2}{2} \right) + \frac{z}{2} \left( 1 + \text{erf} \left( \frac{z}{\sqrt{2}} \right) \right)
$$

(12)

$$
\text{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z \exp(-t^2)dt.
$$

(13)

**Proof.** Please see [65] for a proof. \(\square\)

**Theorem 4.2.** Let $X_{ij} \sim \sum_{k=1}^{K} \pi_k N(M^{[k]}_{ij}, S^{[k]}_{ij})$. Given the aggregation matrix $L$ and the weight matrix $W$, then:

$$
\text{ReLU}(LXW)_{ij} = \sum_{k=1}^{K} \pi_k \sqrt{S_{ij}^{[k]}} \text{NR} \left( \hat{\mu}_{ij}^{[k]} \right)
$$

(14)

$$
\text{LeakyReLU}(LXW)_{ij} = \sum_{k=1}^{K} \pi_k \left( \sqrt{S_{ij}^{[k]}} \text{NR} \left( \hat{\mu}_{ij}^{[k]} \right) - \alpha \sqrt{S_{ij}^{[k]}} \text{NR} \left( \hat{\mu}_{ij}^{[k]} \right) \right).
$$

(15)

where $\odot$ is element-wise multiplication, $\alpha$ is the negative slope parameter of LeakyReLU activation, and

$$
\hat{M}^{[k]} = LM^{[k]} W
$$

(16)

$$
\hat{S}^{[k]} = (L \odot L)S^{[k]} (W \odot W).
$$

(17)

**Proof.** The element of matrix $LXW$ can be expressed as:

$$
(LXW)_{ij} = \sum_{d=1}^{D} \sum_{n=1}^{N} L_{in} X_{nd} W_{dj}
$$

(18)

Based on the property of Gaussian distribution, $(LXW)_{ij}$ also follows a mixture of Gaussian distributions as:

$$
\sum_{k=1}^{K} \pi_k \mathcal{N} \left( \sum_{d=1}^{D} \sum_{n=1}^{N} L_{in} M_{nd}^{[k]} W_{dj}, \sum_{d=1}^{D} \sum_{n=1}^{N} L_{in}^2 S_{nd}^{[k]} W_{dj}^2 \right)
$$

(19)

$$
= \sum_{k=1}^{K} \pi_k \mathcal{N} \left( \left( L \odot L \right) S^{[k]} (W \odot W)_{ij} \right)
$$

(20)

$$
= \sum_{k=1}^{K} \pi_k \mathcal{N} \left( \hat{M}_{ij}^{[k]}, \hat{S}_{ij}^{[k]} \right).
$$

(21)

Finally, using the result of Lemma 4.1, we can derive Eq. (14) as:

$$
\text{ReLU}[LXW]_{ij} = \sum_{k=1}^{K} \pi_k \text{ReLU} \left[ \mathcal{N} \left( \hat{M}_{ij}^{(k)}, \hat{S}_{ij}^{(k)} \right) \right]
$$

(22)

$$
= \sum_{k=1}^{K} \pi_k \sqrt{\hat{S}_{ij}^{[k]}} \text{NR} \left( \hat{M}_{ij}^{[k]} \right).
$$

(23)

Eq. (15) can be proved similarly and the proof is omitted due to lack of space. \(\square\)

Thus, we can calculate the expected activation of neurons for the first layer according to Theorem 4.2. Calculation of the subsequent layers remain unchanged.

### 4.3 The Network Architecture

Our approach is named GCNMF. We illustrate the model architecture in Figure 1 and provide the following explanations.

- **Initialize the hyper-parameters**
  The additional hyper-parameters include the number of layers $L$, the number of Gaussian components $K$.

- **Initialize the model parameters**
  The model parameters include GMM parameters $(\pi_k, \mu^{[k]}, \Sigma^{[k]})$ and conventional network parameters. GMM parameters are initialized by EM algorithm [19] that explores the data density $d$.

- **Forward propagation**
  Calculate the first layer according to Theorem 4.2, and calculate the other layers as usual.

- **Backward propagation**
  Apply gradient descent optimization algorithms to jointly learn the GMM parameters and network parameters by minimizing a cost function that is created based on a specific task.

- **Consistency**
  GCNMF is consistent with GCN when the features are complete. Suppose $S = 0$. It follows that $\sigma[(LXW)_{ij}] = \sigma((LXW)_{ij})$.

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1The algorithm implementation is provided by scikit-learn: https://scikit-learn.org/
We conducted experiments on the node classification task to answer the following questions:

- Does GCN\textsuperscript{MF} agree with our intuition and perform well?
- Where do imputation based methods fail?
- Is GCN\textsuperscript{MF} sensitive to the hyper-parameters?
- Is GCN\textsuperscript{MF} computationally expensive?

In the following, we first explain experimental settings in detail, including baselines and datasets. After that, we discuss the results.

### Time Complexity

In the following, we analyze the time complexity of the forward propagation. Note that GCN\textsuperscript{MF} modifies the original GCN in the first layer, where the calculation of Eq. (1) is replaced by Eq. (14) or (15). We assume that L is a sparse matrix. The calculation of Eq. (1) takes $O(|E|D + NDD^{(1)})$ complexity [15].

Eq. (14) or (15) requires calculation of Eq. (16) and (17). The complexity of Eq. (16) for all $k$ is $O(K(|E|D + NDD^{(1)}))$. The complexity of Eq. (17) for all $k$ is $O(|E|) + O(DD^{(1)}) + O(K(|E|D + NDD^{(1)}))$, where the first two terms are for ($L \odot L$) and ($W \odot W$), respectively. Given $\tilde{S}_{ij}^{(k)}$ and $\hat{M}_{ij}^{(k)}$, Eq. (14) or (15) takes $O(KND^{(1)})$ time for all $i, j$.

Putting them all together, the total complexity of the first layer of GCN\textsuperscript{MF} is $O(K(|E|D + NDD^{(1)})) + O(|E|) + O(DD^{(1)}) + O(K(|E|D + NDD^{(1)})) + O(KND^{(1)}) = O(K(|E|D + NDD^{(1)}))$. Since the number of components $K$ is usually small, the forward propagation of GCN\textsuperscript{MF} has the same complexity as GCN.

### 5 EXPERIMENTS

We conducted experiments on the node classification task to answer the following questions:

- Does GCN\textsuperscript{MF} agree with our intuition and perform well?
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### Datasets

We did experiments on four real-world graph datasets that are commonly used. Descriptions of these graphs are as follows and Table 1 summarizes their statistics.

- Cora and Citeseer [60]: The citation graphs, where nodes are documents and edges are citation links. Node features are bag-of-words representations of documents. Each node is associated with a label representing the topic of documents.
- AmaPhoto and AmaComp [47]: The product co-purchase graphs, where nodes are products and edges exist between products that are co-purchased by users frequently. Node features are bag-of-words representations of product reviews. Node labels represent the category of products.

We pre-processed the datasets and removed some features concerning two cases.

- **Randomly missing features**
  - The features are missing at random. Specifically, $S$ was randomly selected with uniform probability.
- **Structurally missing features**
  - The features do not exist for some nodes. Specifically, $V' \subseteq V$ was randomly selected, and then $S = \{(i, j)|v_i \in V', j = 1, \ldots, D\}$.

### Baselines

We consider the following imputation methods to fill in missing values and then apply GCN on the complete graphs.

- **MEAN [24]**: This method replaces missing values with the mean of observed features.
- **K-NN [6]**: This approach samples similar features by $k$-nearest neighbors and then replaces missing values with the mean of these features. We set $k = 5$.
- **MFT [38]**: This is the imputation method based on factorizing the incomplete matrix into two low-rank matrices.
- **SOFTIMP [46]**: This method estimates missing values by soft-thresholded singular value decomposition (SVD).
- **MICE [9]**: This is the multiple imputation method that infers missing values from the conditional distributions by Markov chain Monte Carlo (MCMC) techniques.
- **MissForest [69]**: This is a non-parametric imputation method that utilizes Random Forest to predict missing values.
- **VAE [36]**: This is a VAE based method for reconstructing missing values.
- **GAIN [93]**: This is a GAN-based approach for imputing missing data.
- **GINN [67]**: This is an imputation method based on graph denoising autoencoder.

### Table 1: Statistics of datasets.

| Dataset     | #Nodes | #Edges | #Features | #Classes | #Train nodes | #Validation nodes | #Test nodes |
|-------------|--------|--------|-----------|----------|--------------|------------------|-------------|
| Cora        | 2,708  | 5,429  | 1,433     | 7         | 140          | 500              | 500         |
| Citeseer    | 3,327  | 4,732  | 3,703     | 8         | 120          | 500              | 500         |
| AmaPhoto    | 7,650  | 143,663| 745       | 10        | 320          | 500              | 500         |
| AmaComp     | 13,752 | 287,209| 767       | 10        | 400          | 500              | 500         |
| **Total**   | 20,041 | 331,001| 2,185     | 27        | 600          | 1,500            | 1,000       |

### Time Complexity

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In the following, we first explain experimental settings in detail, including baselines and datasets. After that, we discuss the results.
### Table 2: The average accuracy in Cora.

| Missing type | Missing rate | 10% | 20% | 30% | 40% | 50% | 60% | 70% | 80% | 90% |
|--------------|--------------|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| Randomly Missing | MEAN | 80.96 | 80.41 | 79.48 | 78.51 | 77.17 | 73.66 | 56.24 | 20.49 | 13.22 |
| | K-NN | 80.45 | 80.10 | 78.86 | 77.26 | 75.34 | 71.55 | 66.44 | 40.99 | 15.11 |
| | MFT | 80.70 | 80.03 | 78.97 | 78.12 | 76.43 | 71.33 | 45.82 | 27.22 | 23.98 |
| | SoftImp | 80.74 | 80.32 | 79.65 | 78.68 | 77.32 | 74.26 | 70.36 | 64.93 | 41.20 |
| | MICE | – | – | – | – | – | – | – | – | – |
| | MissForest | 80.68 | 80.43 | 79.74 | 79.27 | 76.12 | 73.70 | 68.31 | 60.92 | 45.89 |
| | VAE | 80.91 | 80.47 | 79.18 | 78.38 | 76.84 | 72.41 | 50.79 | 18.12 | 13.27 |
| | GAIN | 80.43 | 79.72 | 78.35 | 77.01 | 75.31 | 72.50 | 70.34 | 64.85 | 58.87 |
| | GINN | 80.77 | 80.01 | 78.77 | 76.67 | 74.08 | 71.66 | 58.42 | 56.21 | 49.04 |
| | GCNmf | 81.70 | 81.66 | 80.41 | 79.52 | 77.91 | 76.67 | 74.38 | 70.57 | 63.49 |
| Performance gain (%) | | | | | | | | | | |
| Structurally Missing | MEAN | 80.91 | 80.41 | 79.52 | 77.91 | 76.67 | 74.38 | 70.57 | 63.49 | 57.63 |
| | K-NN | 80.76 | 80.26 | 78.63 | 77.51 | 74.51 | 70.86 | 63.29 | 37.97 | 13.95 |
| | MFT | 80.91 | 80.34 | 78.93 | 77.48 | 74.47 | 71.33 | 52.65 | 29.96 | 17.05 |
| | SoftImp | 79.71 | 69.47 | 69.31 | 52.53 | 44.71 | 40.07 | 36.68 | 28.51 | 27.98 |
| | MICE | 80.92 | 80.40 | 79.05 | 77.72 | 75.22 | 72.18 | 56.30 | 25.56 | 13.86 |
| | MissForest | 80.48 | 79.88 | 78.54 | 76.93 | 73.88 | 68.13 | 54.29 | 30.82 | 14.05 |
| | VAE | 80.63 | 79.98 | 78.57 | 77.42 | 74.69 | 69.95 | 60.71 | 36.59 | 17.27 |
| | GAIN | 80.53 | 79.78 | 78.36 | 76.97 | 74.25 | 69.90 | 61.33 | 41.09 | 18.43 |
| | GINN | 80.85 | 80.27 | 78.88 | 77.35 | 74.76 | 70.58 | 59.45 | 29.15 | 13.92 |
| | GCNmf | 81.65 | 80.77 | 80.67 | 79.24 | 77.43 | 75.97 | 72.69 | 68.00 | 55.64 |
| Performance gain (%) | | | | | | | | | | |

### Table 3: The average accuracy inCiteseer.

| Missing type | Missing rate | 10% | 20% | 30% | 40% | 50% | 60% | 70% | 80% | 90% |
|--------------|--------------|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| Randomly Missing | MEAN | 69.88 | 69.62 | 68.97 | 65.12 | 54.62 | 37.39 | 18.29 | 12.28 | 11.88 |
| | K-NN | 69.84 | 69.38 | 68.69 | 67.18 | 62.64 | 54.75 | 32.20 | 14.84 | 12.73 |
| | MFT | 69.70 | 69.51 | 68.74 | 65.31 | 60.56 | 41.53 | 34.10 | 17.26 | 19.29 |
| | SoftImp | 69.63 | 69.34 | 69.23 | 68.47 | 66.35 | 65.53 | 60.86 | 52.23 | 31.08 |
| | MICE | – | – | – | – | – | – | – | – | – |
| | MissForest | 69.80 | 69.39 | 68.54 | 64.13 | 50.91 | 29.62 | 14.85 | 12.75 | 11.21 |
| | VAE | 69.64 | 68.88 | 67.56 | 65.97 | 63.86 | 60.74 | 55.77 | 52.05 | 42.73 |
| | GAIN | 70.07 | 69.79 | 68.87 | 68.14 | 63.21 | 43.61 | 20.74 | 13.26 | 11.31 |
| | GINN | 70.93 | 70.82 | 70.67 | 72.24 | 74.43 | 73.97 | 72.69 | 68.00 | 55.64 |
| Performance gain (%) | | | | | | | | | | |
| Structurally Missing | MEAN | 69.08 | 68.40 | 67.05 | 67.73 | 75.22 | 70.18 | 56.30 | 25.56 | 13.86 |
| | K-NN | 69.76 | 69.26 | 68.63 | 67.51 | 74.51 | 70.86 | 63.29 | 37.97 | 13.95 |
| | MFT | 69.91 | 69.34 | 68.79 | 65.31 | 60.56 | 41.53 | 34.10 | 17.26 | 19.29 |
| | SoftImp | 79.71 | 69.47 | 69.31 | 52.53 | 44.71 | 40.07 | 36.68 | 28.51 | 27.98 |
| | MICE | 80.92 | 80.40 | 79.05 | 77.72 | 75.22 | 72.18 | 56.30 | 25.56 | 13.86 |
| | MissForest | 69.48 | 79.88 | 78.54 | 76.93 | 73.88 | 68.13 | 54.29 | 30.82 | 14.05 |
| | VAE | 69.63 | 79.98 | 78.57 | 77.42 | 74.69 | 69.95 | 60.71 | 36.59 | 17.27 |
| | GAIN | 69.53 | 79.78 | 78.36 | 76.97 | 74.25 | 69.90 | 61.33 | 41.09 | 18.43 |
| | GINN | 80.85 | 80.27 | 78.88 | 77.35 | 74.76 | 70.58 | 59.45 | 29.15 | 13.92 |
| | GCNmf | 81.65 | 80.77 | 80.67 | 78.24 | 77.43 | 75.97 | 72.69 | 68.00 | 55.64 |
| Performance gain (%) | | | | | | | | | | |

GCN 81.49

GCN 70.65
## Table 4: The average accuracy in AmaPhoto.

| Missing type | Missing rate | 10% | 20% | 30% | 40% | 50% | 60% | 70% | 80% | 90% |
|--------------|--------------|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MEAN         | 92.15        | 92.05 | 91.81 | 91.62 | 91.40 | 90.76 | 89.88 | 86.41 | 68.88 |
| K-NN         | 92.27        | 92.12 | 91.94 | 91.67 | 91.37 | 90.92 | 90.03 | 87.41 | 81.91 |
| MFT          | 92.23        | 92.07 | 91.88 | 91.51 | 91.15 | 90.11 | 88.28 | 85.17 | 75.73 |
| SoftImp      | 92.23        | 92.09 | 91.92 | 91.78 | 91.55 | 91.18 | 90.55 | 88.93 | 85.22 |
| MICE         | 92.23        | 92.07 | 91.97 | 91.75 | 91.52 | 91.22 | 90.42 | 86.43 | 82.88 |
| MissForest   | 92.18        | 92.09 | 91.82 | 91.61 | 91.42 | 90.71 | 89.17 | 86.03 | 82.82 |
| VAE          | 92.20        | 92.08 | 91.90 | 91.55 | 91.18 | 90.55 | 89.28 | 86.95 | 81.43 |
| GAIN         | 92.23        | 92.11 | 91.90 | 91.73 | 91.49 | 91.24 | 90.72 | 89.49 | 86.96 |
| GINN         | 92.25        | 92.03 | 91.87 | 91.53 | 91.14 | 90.56 | 88.59 | 85.02 | 79.80 |
| GAIN         | 92.23        | 92.44 | 92.20 | 92.09 | 92.09 | 91.69 | 91.25 | 90.57 | 88.96 |
| Performance gain (%) | 0.29 | 0.35 | 0.25 | 0.59 | 0.49 | 0.58 | 1.21 | 2.30 | 29.15 |

## Table 5: The average accuracy in AmaComp.

| Missing type | Missing rate | 10% | 20% | 30% | 40% | 50% | 60% | 70% | 80% | 90% |
|--------------|--------------|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MEAN         | 82.79        | 82.36 | 81.51 | 80.53 | 79.30 | 77.22 | 74.56 | 61.60 | 5.92 |
| K-NN         | 82.89        | 82.73 | 82.18 | 82.00 | 81.54 | 80.58 | 79.34 | 76.81 | 66.04 |
| MFT          | 82.82        | 82.54 | 82.05 | 81.58 | 80.76 | 79.28 | 77.11 | 72.31 | 49.42 |
| SoftImp      | 82.68        | 82.75 | 82.37 | 82.06 | 81.48 | 80.48 | 79.27 | 77.29 | 69.04 |
| MICE         | 82.83        | 82.76 | 82.43 | 82.28 | 81.66 | 80.59 | 78.65 | 75.00 | 63.60 |
| MissForest   | 82.89        | 82.78 | 82.44 | 81.96 | 81.56 | 80.71 | 79.96 | 75.80 | 67.26 |
| VAE          | 82.94        | 82.78 | 82.27 | 81.65 | 80.89 | 79.57 | 78.22 | 76.00 | 71.98 |
| GAIN         | 82.94        | 82.78 | 82.27 | 81.65 | 80.89 | 79.57 | 78.22 | 76.00 | 71.98 |
| GINN         | 82.94        | 82.94 | 82.78 | 82.27 | 81.65 | 80.89 | 79.57 | 78.22 | 76.00 |
| GCM         | 82.45        | 82.32 | 82.08 | 81.88 | 81.52 | 80.89 | 80.39 | 89.64 | 86.09 |
| Performance gain (%) | 0.37 | 0.49 | 0.53 | 0.70 | 0.98 | 0.91 | 1.78 | 4.51 | 6.97 |

## Graph Convolutional Networks for Graphs Containing Missing Features

### Performance gain (%)

| Method      | Randomly Missing | Structurally Missing |
|-------------|------------------|----------------------|
| GCN         | 92.35            | 92.35                |

### Performance gain (%)

| Method      | Randomly Missing | Structurally Missing |
|-------------|------------------|----------------------|
| GCN         | 92.35            | 92.35                |
Experimental Setup. We followed the data splits of previous work [88] on Cora and Citeseer. As for AmaPhoto and AmaComp, we randomly chose 40 nodes per class for training, 500 nodes for validation, and the remaining for testing.

We gradually increased the missing rate $mr$ from 10% to 90%, which is defined as $mr = |S|/(ND)$ for randomly missing features and $mr = |V'|/N$ for structurally missing features. With each missing rate, we generated five instances of missing data and evaluated the performance twenty times for each instance.

To ensure a fair comparison, we employed the following parameter settings of GCN model for all approaches: we set the number of layers to 2, the number of hidden units to 16 (Cora and Citeseer) and 64 (AmaPhoto and AmaComp).

We employed Optuna [2] and carefully tuned the hyper-parameters such as learning rate, $L_2$ regularization, and dropout rate for each approach based on the validation set. We followed the normalized initialization scheme [25] to initialize the weight matrix. We adopted Adam algorithm [35] for optimization, and an early stopping strategy with a patience of 100 epochs to avoid over-fitting [72]. Moreover, we simply set the number of Gaussian components to 5 across all datasets. The implementation of all approaches is in Python and PyTorch and we ran the experiments on a single machine with Intel Xeon Gold 6148 Processor @2.40GHz, NVIDIA Tesla V100 GPU, and RAM @64GB.

For reproducibility, the source code of GCNmf and the graph datasets are publicly available$^2$

5.1 Performance Comparison

Table 2 - Table 5 compare the average accuracy obtained by different methods. Bold and underline indicate the best and the second best score for each setting. The accuracy of GCN in the case of complete features is also provided as a reference. Note that some results of MICE (in Cora and Citeseer) and MissForest (in Citeseer and AmaComp) are not available because we encountered unexpected runtime error or the program takes more than 24 hours to terminate. We have the following observations.

First, GCNmf demonstrates the best performance and there is no method that clearly win the second place. GCNmf achieves the highest accuracy for almost all of the missing rates and across all datasets, with only three exceptions. For the randomly missing case, GCNmf is markedly superior to the others. It achieves improvement of up to 8.6%, 11.82%, 2.30%, and 5.24% when compared with the best accuracy scores among baselines in the four datasets, respectively. For the structurally missing case, this advantage becomes even greater, with the corresponding maximum improvement raising to 99.43%, 102.96%, 6.97%, and 35.36%, respectively. Most strikingly, when missing rate reaches 80%, i.e., the features of 80% nodes are not known, GCNmf can still achieve an accuracy of 68.00% in Cora, while all baselines fail.

Secondly, GCNmf is more appealing when a large portion of features are missing. This can be explained by the fact that the performance gain, on the whole, becomes larger and larger as the missing rate increases. In contrast, the imputation based method becomes less reliable at high missing rates. For example, the accuracy of baselines (except for SortImpute) falls to below 20.0% when missing rate reaches 90% for the structurally missing case in Cora.

Thirdly, it is interesting to note that GCNmf even outperforms GCN when only a small number of features are missing. For example, GCNmf holds a slight advantage over GCN when the missing rate is 10% in the four datasets. This indicates that GCNmf is robust against low-level missing features.

Figure 2 - Figure 4 show the variability of the performance for different methods. We can see that GCNmf is more robust than the baselines, especially in Cora and Citeseer, where there is a high level of variability. Moreover, GCNmf and GCN are on the same level of variability. This implies that representing incomplete features by GMM and calculating the expected activation of neurons do not undermine the robustness of GCN.

We attribute the superiority of GCNmf to the joint learning of GMM and network parameters. Actually, our approach can be understood as calculating the expected activation of neurons over the imputations drawn from missing data density in the first layer. It is the end-to-end joint learning of the parameters that make our approach less likely to converge to sub-optimal solutions.

5.2 Hyper-Parameter Analysis

Next, we study the performance of GCNmf with different assignments of hyper-parameters. Figure 5 depicts the performance with different assignments on the Gaussian components $K$ and the number of hidden units $D^{(1)}$ in Cora and AmaPhoto datasets. We can observe that the performance reaches a plateau when we have enough number of hidden units to transcribe the information, i.e., $D^{(1)} \geq 16$ for Cora and $D^{(1)} \geq 32$ for AmaPhoto. On the other hand, the performance is not sensitive to $K$, with differences between the best and worst less than 0.82% when $D^{(1)} \geq 16$ in Cora and 0.30% when $D^{(1)} \geq 32$ in AmaPhoto, respectively.

5.3 Running Time Comparison

Finally, we compare the running time for different approaches in Table 6. The numbers represent the sum of time for parameter initialization, missing value imputation, and model training. We also provide a reference time of GCN when $S = \emptyset$. We can observe that GCNmf algorithm runs in reasonable time, with model training taking the majority of time (the time for initialization of GMM parameters only accounts for less than 25%). In comparison, GCNmf is slower than MEAN and VAE, but is much faster than the other seven methods. We note that some imputation techniques suffer due to the high dimension of features. For example, MissForest did not finish within 24 hours in Citeseer.

6 CONCLUSION

We proposed GCNmf to supplement a severe deficiency of current GCN models—inability to handle graphs containing missing features. In contrast to the traditional strategy of imputing missing features before applying GCN, GCNmf integrates the processing of missing features and graph learning within the same neural network architecture. Specifically, we propose a novel way to unify the representation of missing features and calculation of the expected

$^2$https://github.com/marblet/GCNmf
Graph Convolutional Networks for Graphs Containing Missing Features

activation of the first layer neurons in GCN. We empirically demonstrate that 1) GCNmf is robust against low level of missing features, 2) GCNmf significantly outperforms the best imputation based methods by up to 99.43%, 102.96%, 6.97%, 35.36% in four benchmark graphs when a large portion of features are missing.

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Table 6: The running time (seconds) of different approaches in the randomly missing case \((mr = 50\%)\). The figure in the parentheses indicates the time for initialization of GMM parameters.

|           | Cora  | Citeseer | AmaPhoto | AmaComp |
|-----------|-------|----------|----------|---------|
| MEAN      | 1.10  | 1.24     | 12.09    | 14.14   |
| K-NN      | 125.04| 480.19   | 482.73   | 1505.14 |
| MFT       | 141.14| 567.50   | 428.95   | 906.52  |
| SoftIMP   | 115.15| 850.55   | 59.26    | 95.14   |
| MICE      | –     | –        | 3879.59  | 6705.73 |
| MissForest| 4039.10| 32528.25| 48264.58 |
| VAE       | 7.91  | 8.64     | 14.23    | 18.78   |
| GAIN      | 79.35 | 426.10   | 36.06    | 35.19   |
| GINN      | 300.64| 839.96   | 998.03   | 3199.96 |
| GCNMF     | 7.43 (0.59) | 13.52 (2.60) | 22.64 (4.11) | 42.38 (9.75) |

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