Graph Encoder Embedding

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Abstract—In this paper we propose a lightning fast graph embedding method called graph encoder embedding. The proposed method has a linear computational complexity and the capacity to process billions of edges within minutes on standard PC — an unattainable feat for any existing graph embedding method. The speedup is achieved without sacrificing embedding performance: the encoder embedding performs as good as, and can be viewed as a transformation of the more costly spectral embedding. The encoder embedding is applicable to either adjacency matrix or graph Laplacian, and is theoretically sound, i.e., under stochastic block model or random dot product graph, the graph encoder embedding asymptotically converges to the block probability or latent positions, and is approximately normally distributed. We showcase three important applications: vertex classification, vertex clustering, and graph bootstrap; and the embedding performance is evaluated via a comprehensive set of synthetic and real data. In every case, the graph encoder embedding exhibits unrivalled computational advantages while delivering excellent numerical performance.

Index Terms—Graph Embedding, Graph Laplacian, Random Dot Product Graph, Central Limit Theorem, Vertex Clustering, Vertex Classification

1 INTRODUCTION

Graph data has gained many recent interests due to its special structure. It arises naturally in modern data, captures interactions among objects, and often sheds valuable insights into the subsequent inference. Given \( n \) vertices and \( s \) edges, a graph can be conveniently represented by an \( n \times n \) adjacency matrix \( A \) where \( A(i, j) \) denotes the edge between \( i \)th vertex and \( j \)th vertex. Equivalently but more succinctly, real graphs are almost always stored by an \( s \times 3 \) edgelist \( E \), where the first two columns store the vertex indices of each edge and the last column stores the edge weight. Examples include social networks, brain regions, article hyperlinks [1], [2], [3], [4], [5], etc.

The unique high-dimensional structure of graph data poses brand new challenges to graph inference problems. To better utilize graph data, graph embedding is the most popular and common approach, i.e., it learns a low-dimensional Euclidean representation of each vertex, such that subsequent inferences can be directly performed on the vertex embedding. The spectral embedding method [6], [7], [8], [9], [10], [11], [12] is arguably the most well-studied graph embedding method in the statistics community: by using singular value decomposition (SVD) on graph adjacency or graph Laplacian, the resulting vertex embedding asymptotically converges to the block probability or latent positions under stochastic block model or random dot product graph, and is approximately normally distributed. We showcase three important applications: vertex classification, vertex clustering, and graph bootstrap; and the embedding performance is evaluated via a comprehensive set of synthetic and real data. In every case, the graph encoder embedding exhibits unrivalled computational advantages while delivering excellent numerical performance.

However, all aforementioned graph embedding methods require some tuning parameters, are computationally expensive, and do not scale well to big graph. Both spectral embedding and GCN require \( \mathcal{O}(n^2) \) in running time and storage complexity, thus unfeasible for millions of vertices without special computation tools. Node2vec does scale linearly with the number of vertices but incurs a very large constant due to the algorithm design, e.g., it takes about 4 hours to process 1M vertices and 10M edges [13]. As modern social networks may easily have billions of edges, a more scalable embedding solution is direly needed.

Towards that target, we propose and investigate the graph encoder embedding in this paper. The graph encoder embedding does not need tuning parameter, has a linear computational complexity and storage requirement, is applicable to either the adjacency matrix or graph Laplacian, and is capable of processing billions of edges within minutes on a standard PC. Moreover, the graph encoder embedding enjoys similar theoretical properties as the spectral embedding; the encoder embedding asymptotically converges to the block probability or latent positions under stochastic block model or random dot product graph, and is approximately normally distributed. We showcase three applications in this paper: vertex classification, vertex clustering, and graph bootstrap. Comprehensive experiments on synthetic and real graphs are carried out to demonstrate its excellent performance. As a result, the graph encoder embedding provides a great tool to better explore, visualize, and interpret network communities in graph of any size. All proofs and simulation function details are in the Appendix. Matlab and Python code are made available on Github.

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1. https://github.com/cshen6/GraphNN
2 Method

Graph Encoder Embedding (GEE)

Algorithm 1 presents the graph encoder embedding when some vertex labels are known. The inputs are: an edgelist $E_i$; a label vector $Y_k$ of $K$ classes, where known labels lie in $\{1, \ldots, K\}$ and unknown labels are set to 0; a Boolean variable $Lap$ stating whether graph Laplacian or graph adjacency is used. The outputs are the projection matrix $W$ and final embedding $Z$. The $i$th column of $Z$ is denoted by $Z_i$, which is the encoder embedding for the $i$th vertex.

Algorithm 1 Graph Encoder Embedding

Require: An edgelist $E \in \mathbb{R}^{s \times 3}$, the corresponding class label $Y \in \{0, \ldots, K\}^n$, and a Boolean variable $Lap$.
Ensure: The encoder embedding $Z \in \mathbb{R}^{K \times n}$, and the projection matrix $W \in \mathbb{R}^{n \times K}$.

function GEE($E, Y, lap$)

if Lap=true then

$D = \text{zeros}(n, 1)$; \hspace{1em} \text{\small degree vector}
for $i = 1, \ldots, n$ do

$D(E(i, 1)) = D(E(i, 1)) + 1;$
$D(E(i, 2)) = D(E(i, 2)) + 1;$
end for

end if

for $k = 1, \ldots, K$ do

$\text{ind} = \text{find}(Y = k);$ \hspace{1em} \text{\small find indices of class k}
$\text{n}_k = \text{sum}(\text{ind});$
$W(\text{ind}, k) = 1/\text{n}_k;$
end for

for $i = 1, \ldots, s$ do

$a = E(i, 1); b = E(i, 2);$
$c = Y(a); d = Y(b); e = E(i, 3);$
$Z(a, d) = Z(a, d) + W(b, d) * e;$
$Z(b, c) = Z(b, c) + W(a, c) * e;$
end for

end function

The algorithm is applicable to any graph, including directed or weighted graph. It is also applicable to an adjacency matrix input $A$ by transforming the adjacency matrix to an edgelist. To operate on graph Laplacian, the method computes the degree vector and applies it to the edge weights, which is equivalent to $D^{-0.5}AD^{-0.5}$ in matrix form where $D$ is the $n \times n$ degree matrix. Next, calculate $n_k$ as the number of vertices in each class, and constructs the matrix $W$ — which is essentially a 0/1 projection matrix normalized by the number of vertices in each class. The final embedding $Z$ is a linear projection of the adjacency or Laplacian matrix onto the subspace $W$ spans.

Algorithm 1 assumed at least some vertices have known labels. This is often the case in practice and a natural setup for vertex classification, which is evaluated in-depth in Section 5. Then Section 6 and Algorithm 2 consider the case where no label information is given.

We call the encoder embedding using adjacency as the adjacency encoder embedding (AEE), and the Laplacian version as the Laplacian encoder embedding (LEE). They may be viewed as a transformation of the adjacency / Laplacian spectral embedding (ASE / LSE). Graph adjacency and graph Laplacian has their own unique properties as summarized in [12], unless mentioned otherwise, by default we assume that the graph encoder embedding uses the adjacency matrix in this paper.

Computational Advantages

Algorithm 1 has a computational complexity and storage requirement of $O(nK + s)$. As $s$ typically far exceeds $nK$, the complexity scales linearly with the number of edges. As most real graphs are sparse with $s = O(n)$, it also scales linearly with number of vertices for sparse graphs.

The running time advantage is demonstrated in Figure 1 comparing four methods: the encoder embedding using edgelist input, the encoder embedding using matrix input, the spectral embedding, and graph convolutional network. The encoder embedding is much faster than other methods: it takes a mere 6 seconds to process 10 million edges, while node2vec required 4 hours [13] and spectral embedding or GCN cannot be run on standard PC for such graphs. At 100 million edges, encoder embedding runs in a minute; and at 1 billion edges with 10M vertices, we reached the maximum memory space a top-end PC can handle, yet graph encoder embedding process data in just 10 minutes. This makes graph encoder embedding the fastest and most scalable graph embedding approach thus far.

3 Theorems

In this section we first review three arguably most popular random graph models, then present the supporting theorems for the graph encoder embedding. For ease of presentation, we assume $n$ is the number of vertices with known labels in all theorems.

Stochastic Block Model (SBM)

SBM is arguably the most fundamental community-based random graph model to generate a graph [15], [16], [17], denoted by $A \sim \text{SBM}(B)$.

Each vertex $i$ is associated with a class label $Y_i \in \{1, \ldots, K\}$ (i.e., communities). The class label may be fixed a-priori, or generated by a categorical distribution with prior probability $\{\pi_k \in (0, 1) \text{ for } k = 1, \ldots, K \text{ satisfying } \sum_k \pi_k = 1\}$.

The block probability matrix $B = [B(k, l)] \in [0, 1]^{K \times K}$ specifies the edge probability between a vertex from class $k$ and a vertex from class $l$: for any $i < j$, $A(i, j) \overset{i.i.d.}{\sim} \text{Bernoulli}(B(Y_i, Y_j))$, $A(i, i) = 0$, $A(j, i) = A(i, j)$.

SBM graph is symmetric and binary with no self-loop.
Fig. 1. Generate random graphs with $K = 5$, average degree 100, and increasing sample size to measure the running time. We report the average running time of each embedding method using 50 Monte Carlo replicates. The top two panels increases the number of vertices from 1000 to 20,000. The left panel uses graph adjacency while the right panel uses the graph Laplacian. The bottom panel increases the number of edges from $10^4$ to $10^9$, and only includes the encoder embedding as other methods do not scale to huge graphs.

Degree-Corrected Stochastic Block Model (DC-SBM)

The DC-SBM graph is a generalization of SBM to better model the sparsity of real graphs [18], denoted by $A \sim \text{DC-SBM}(B, \{\theta_i\})$.

Everything else being the same as SBM, each vertex has an additional degree parameter $\{\theta_i\}$. Then the adjacency matrix is generated by

$$ A(i, j) \sim \text{Bernoulli}(\theta_i \theta_j B(Y_i, Y_j)) $$

for any $i < j$. The degree coefficients typically require certain constraints for the above to be a valid probability. In this paper we simply assume

$$ \theta_i \overset{i.i.d.}{\sim} F_\theta \in (0, M]. \tag{1} $$

Namely, the degree coefficient is non-trivial and bounded, which is a very general assumption. When $\theta_i = 1$ for all $i$, DC-SBM becomes SBM.

Random Dot Product Graph (RDPG)

Another popular random graph model is RDPG [19], denoted by $A \sim \text{RDPG}(\{X_i\})$. Under RDPG, each vertex $i$ is associated with a latent position vector $X_i \overset{i.i.d.}{\sim} F_X \in [0, 1]^p$ for $i = 1, \ldots, n$. Then for any $i < j$,

$$ A(i, j) \sim \text{Bernoulli}(X_i^T X_j), $$

$$ A(i, i) = 0, \quad A(j, i) = A(i, j). $$

Typically $F_X$ is constrained with $X_i^T X_j \in (0, 1]$, i.e., the inner product shall be a valid and nontrivial probability.

To generate RDPG graph with communities, it suffices to use a K-component mixture distribution. Namely, let $(X_i, Y_i) \overset{i.i.d.}{\sim} F_{XY} \in \mathbb{R}^p \times [K]$, where $Y_i$ is the class label in $[1, 2, \ldots, K]$.

Asymptotic Convergence

Theorem 1. Suppose $A \sim \text{SBM}(B)$. For a given $i$th vertex of class $y$, its graph encoder embedding $Z_i$ converges to the respective block probability vector:

$$ \|Z_i - B(:, y)\|_2 \overset{n \to \infty}{\longrightarrow} 0. $$

Theorem 2. Suppose $A \sim \text{DC-SBM}(B, \{\theta_j\})$. For a given $i$th vertex of class $y$, its graph encoder embedding $Z_i$ converges to the block probability vector up-to the degree coefficients:

$$ \|Z_i - \theta_i \cdot B(:, y) \otimes \bar{\Theta}\|_2 \overset{n \to \infty}{\longrightarrow} 0, $$

where $\bar{\Theta} = [\bar{\theta}_1, \cdots, \bar{\theta}_K] \in \mathbb{R}^K$ and $\bar{\theta}_k = E(\theta_i | Y_i = k)$ denotes the class-conditional mean of vertex degrees, and $\otimes$ denotes the entry-wise multiplication.

Theorem 3. Suppose $A \sim \text{RDPG}(\{X_i\})$. For a given $i$th vertex with an associated latent position $x_i \in \mathbb{R}^p$, its graph encoder embedding $Z_i$ converges to the latent position multiplied by the class-conditional means:

$$ \|Z_i - \lambda_i^T x_i\|_2 \overset{n \to \infty}{\longrightarrow} 0, $$

where $\lambda = [\lambda_1, \lambda_2, \cdots, \lambda_K] \in \mathbb{R}^p \times K$ and $\lambda_k = E(X | Y = k)$ in $\mathbb{R}^p$ denotes the class-conditional mean of the latent variable.

Namely, the graph encoder embedding asymptotically equals: the block probability vector under SBM; the block probability times degree then entry-wise multiplied by the class-conditional degree means under DC-SBM; and the latent variable multiplied by the class-conditional means under RDPG. As a result, the encoder embedding is very informative and interpretable under each model, see Figures 2 - 6 for numerical examples. Therefore, the encoder embedding may be viewed as a transformation of the spectral embedding, because the spectral embedding also estimates the block probability or latent variable up-to rotation [6], [7].

Asymptotic Normality

Moreover, the encoder embedding is approximately normally distributed. To state the central limit result under each case, we introduce some additional notations:

- Define $\bar{\eta} = [\eta_1, \eta_2, \cdots, \eta_n] \in \mathbb{R}^K$, and $\text{Diag}(\cdot)$ as the diagonal matrix of a vector.
- Under SBM with block matrix $B$, define $\Sigma_B(\cdot, y)$ as the $K \times K$ diagonal matrix with

$$ \Sigma_B(\cdot, y)(k, k) = B(k, y)(1 - B(k, y)) \in \mathbb{R}^{1 \times 1}. $$

- Under DC-SBM with $\{\theta_j \overset{i.i.d.}{\sim} F_\theta\}$, define $\tilde{\theta}_k^2$ as the class-conditional mean of the squared vertex degrees:

$$ \tilde{\theta}_k^2 = E(\theta_j^2 | Y = k), \quad \bar{\Theta}^2 = [\tilde{\theta}_1^2, \tilde{\theta}_2^2, \cdots, \tilde{\theta}_K^2] \in \mathbb{R}^K. $$

• Under RDPG where \((X, Y) \sim F_{XY} \in \mathbb{R}^p \times [K]\) is the latent distribution, define
  \[
  \bar{\lambda}_1(x_i) = E^2(X^T x_i | Y = k), \\
  \bar{\lambda}_2(x_i) = [\bar{\lambda}_1(x_i), \bar{\lambda}_2(x_i), \ldots, \bar{\lambda}_K(x_i)] \in \mathbb{R}^K
  \]
  for any fixed vector \(x_i \in \mathbb{R}^p\).

**Theorem 4.** The graph encoder embedding is asymptotically normally distributed under SBM, DC-SBM, or RDPG. Specifically, as sample size increases, for a given \(i\)th vertex we have

- **under SBM Graph:**
  \[
  \text{Diag}(\bar{\eta})^{0.5} \cdot (Z_i - B(:,y)) \xrightarrow{d} \mathcal{N}(0, \Sigma_{B(:,y)});
  \]

- **under DC-SBM Graph:**
  \[
  \text{Diag}(\bar{\eta})^{0.5} \cdot (Z_i - \theta_i B(:, y) \otimes \bar{\Theta}) \xrightarrow{d} \mathcal{N}(0, \theta_i^2 \text{Diag}(\bar{\Theta}^2). \Sigma_{B(:,y)});
  \]

- **under RDPG Graph:**
  \[
  \text{Diag}(\bar{\eta})^{0.5} \cdot (Z_i - \lambda^T x_i) \xrightarrow{d} \mathcal{N}(0, \text{Diag}(\lambda^T x_i - \lambda^2(x_i))).
  \]

Namely, under SBM, every vertex embedding within the same class is asymptotically identically distributed as the same normal distribution; under DC-SBM, the within-class vertex embedding has the same distribution up-to scaling by its degree; under RDPG, each vertex embedding distributes somewhat differently from each other, where the mean and variance are conditioned on the latent position.

### 4 Embedding Visualization

**Embedding Comparison**

Figure 2 compares the graph encoder embedding to the adjacency spectral embedding under SBM, DC-SBM, and RDPG graph respectively at \(K = 2\). While both embedding methods exhibit clear community separation, the encoder embedding offers better interpretability for the model parameters in each case. For example, under the SBM graph, the encoder embedding centers around the block probability vectors \((0.13, 0.1)\) and \((0.1, 0.13)\) respectively and appears normally distributed within each class; and for the DC-SBM graph, the encoder embedding lies along the block probability vectors scaled by the degree of each vertex.

**Normality Visualization**

Figure 3 presents the graph encoder embedding for a variety of two-class SBM, DC-SBM, and RDPG graphs. To better visualize the normality and make sure each vertex has the same distribution, we plot the degree-scaled embedding for the DC-SBM graphs, i.e., compute \(Z_i / \theta_i / \bar{\Theta}\) (where \(\div\) denotes the entry-wise division); and plot a normalized encoder embedding for the RDPG graphs, i.e., normalize \(Z_i\) by the mean and variance from Theorem 4, then add 0.2 to all class 2 vertices for clearer community separation.

Then we draw two normality circles in every panel, using the class-conditional means as the center and three standard deviation from Theorem 4 as the radius. Figure 3 clearly shows that the graph encoder embedding is approximately normally distributed in every case.
Real Graph Visualization

The graph encoder embedding is equally informative for real graphs, as shown in Figure 4 for the Political Blogs [2] (1490 vertices with 2 classes) and the Gene Network [20] (1103 vertices with 2 classes). For each graph, the vertices are embedded into the two-dimensional Euclidean space. Since the x-axis stands for the first dimension as well as the connectivity to class 1 (and y-axis for class 2), we observe that the vertex embedding appears similar to DC-SBM, thus can be viewed as estimating the block probability scaled by degree. Both real graphs have the property that within-class vertices are better connected than between-class vertices, and the two classes are well-separated except a few outlier vertices that mingle into the other community.

Classification Evaluation on Real Graphs

We downloaded seven real graphs with labels, including four graphs from network repository² [20]: Cora Citations (2708 vertices with 7 classes), Gene Network (1103 vertices with 2 classes), Industry Partnerships (219 vertices with 3 classes), Pubmed Citations (19717 vertices with 3 classes); and three more graphs from Stanford network data³: EU Email Network [21] (1005 vertices with 42 classes), LastFM Asia Social Network [22] (7624 vertices with 17 classes), and Political Blogs [2] (1490 vertices with 2 classes).

For each data and each method, we carried out 10-fold evaluation and report the average classification error and running time in Table 1. The results validate the numerical advantages of graph encoder embedding; in every case, AEE achieves similar error as ASE with a fraction of running time, and often slightly better than spectral embedding; so is LEE vs LSE. Note that the running time includes both embedding and classification; and the running time for encoder embedding mostly comes from the classification step.

Classification Evaluation on Synthetic Data

Figure 5 reports the average 10-fold classification error (i.e., 90% vertices for training and 10% for testing) and average running time, for increasing sample size of simulated SBM, DC-SBM, and RDPG graphs (K = 3) with 100 Monte-Carlo replicates. We compare the adjacency encoder embedding (AEE) with adjacency spectral embedding (ASE) and Laplacian spectral embedding (LSE). We use sparse SVD implementation for both spectral embedding methods. Each embedding method is coupled with two standard classifiers: the linear discriminant analysis (LDA) and the 5-nearest-neighbor (5NN).

As sample size increases, every method has better classification error at the cost of higher running time. In every case, AEE performed very well with much better running time: the encoder embedding has the lowest classification error under SBM, is among the lowest under DC-SBM and RDPG, and only requires a fraction of running time vs spectral embedding.

5 VERTEX CLASSIFICATION

An immediate and important use case herein is vertex classification. The encoder embedding from Algorithm 1 can be directly utilized for subsequent vertex classification, i.e., the vertex embedding with known class labels are the training data, while the vertex embedding with unknown labels are the testing data. For evaluation in this paper, we consider linear discriminant analysis (LDA) and k-nearest-neighbor (kNN) classifiers. One could use any other standard classifier, e.g., logistic regression, random forest, neural network, which all resulted in the same numerical interpretations.

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2. http://networkrepository.com/
3. https://snap.stanford.edu/
6 No Label and Vertex Clustering

To handle graph data with no known labels, we utilize random initialization and k-means clustering to propose an iterative version of encoder embedding in Algorithm 2. The running time is $O(M(nK^2 + s))$, which is also linear with respect to the number of edges but takes more time than Algorithm 1 due to the k-means step and iteration. In our experiments we set the iteration number to $M = 20$, which achieved satisfactory performance.

Algorithm 2 Encoder Embedding for No Known Labels and Vertex Clustering

Require: An edgelist $E$, number of clusters $K$, and iteration limit $M$.
Ensure: The encoder embedding $Z \in \mathbb{R}^{K \times n}$ for all vertices, and the estimated class label $Y \in \{1, \ldots, K\}^n$.

function GEE $\circ$ CLUSTERING($E, K, M$)
    $Y_{new} = \text{rand}(K, n)$;  \text{randomize a label vector}
    for $i = 1, \ldots, M$ do
        $Z = \text{GEE}(E, Y_{new})$;
        $Y = \text{kmeans}(Z, K)$;
        if $\text{ARI}(Y_{new}, Y) == 1$ then
            Stop;
        end if
    end for
end function

As long the sample size is not too small, Algorithm 2 generally performs similar to the partial label case. Just like the classification performance in Section 5, the clustering performance of encoder embedding is also similar to that of spectral embedding in a fraction of running time. Figure 6 provides an illustration of the clustering performance (measured by the adjusted rand index between the clustered indices and true community indices; the larger the better with 1 being perfect clustering) under 3-class SBM and RDPG graphs: the adjacency encoder embedding produces excellent clustering results, which is similar to ASE clustering (ASE followed by k-means) in ARI but much faster. The phenomenon is consistent throughout our synthetic and real graphs.

|     | AEE $\circ$ 5NN | AEE $\circ$ LDA | LEE $\circ$ 5NN | LEE $\circ$ LDA | ASE $\circ$ 5NN | ASE $\circ$ LDA | AEE $\circ$ LDA | LSE $\circ$ 5NN | LSE $\circ$ LDA |
|-----|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|
| Cora| 40.3%          | 51.9%         | 40.7%         | 51.3%         | 52.0%          | 63.7%          | 51.9%         | 65.9%         |
| Email| 41.9%          | 42.8%         | 41.3%         | 42.2%         | 38.8%          | 46.9%          | 70.2%         | 80.5%         |
| Gene| 39.5%          | 24.3%         | 32.5%         | 23.2%         | 33.9%          | 31.6%          | 33.0%         | 31.7%         |
| Industry| 53.7%      | 38.3%         | 50.6%         | 37.4%         | 49.9%          | 38.8%          | 49.9%         | 38.3%         |
| LastFM| 35.6%         | 43.7%         | 33.9%         | 42.8%         | 37.5%          | 54.2%          | 39.0%         | 68.2%         |
| PubMed| 34.5%         | 43.8%         | 34.7%         | 43.2%         | 38.2%          | 54.4%          | 39.8%         | 68.6%         |
| PolBlog| 9.5%          | 10.7%         | 6.3%          | 6.6%          | 5.1%           | 6.4%           | 4.3%          | 4.4%          |

Running Time (seconds)

|     | AEE $\circ$ 5NN | AEE $\circ$ LDA | LEE $\circ$ 5NN | LEE $\circ$ LDA | ASE $\circ$ 5NN | ASE $\circ$ LDA | AEE $\circ$ LDA | LSE $\circ$ 5NN | LSE $\circ$ LDA |
|-----|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|
| Cora| 0.04           | 0.04           | 0.09           | 0.09           | 0.72           | 0.73           | 1.58           | 1.59           |
| Email| 0.01           | 0.25           | 0.02           | 0.27           | 0.06           | 0.30           | 0.17           | 0.41           |
| Gene| 0.01           | 0.01           | 0.01           | 0.01           | 0.05           | 0.05           | 0.08           | 0.08           |
| Industry| 0.01        | 0.01           | 0.01           | 0.01           | 0.02           | 0.02           | 0.02           | 0.02           |
| LastFM| 0.25          | 0.29           | 0.65           | 0.67           | 5.4            | 5.4            | 20.3           | 20.3           |
| PubMed| 0.25          | 0.28           | 0.60           | 0.62           | 5.0            | 5.0            | 19.5           | 19.5           |
| PolBlog| 0.01         | 0.01           | 0.02           | 0.02           | 0.09           | 0.09           | 0.21           | 0.21           |

The 10-fold classification results for seven real graphs. For each row, the lowest classification error / running time is highlighted in bold.
7 GRAPH BOOTSTRAP

Bootstrap is a popular statistical method for resampling Euclidean data [23]. Graph bootstrap, however, remains under-investigated. A naive graph bootstrap procedure can be carried out as follows: simply resample the vertex index with replacement, then re-index both the row and column of the adjacency matrix.

Since the graph encoder embedding offers a good estimate of the block probability, it can provide an elegant and better graph bootstrap solution as detailed in Algorithm 3: given the adjacency matrix and label vector, we compute the encoder embedding and carry out standard bootstrap on the embedding, then use Bernoulli random variable to form the resampled adjacency matrix. We validate the procedure via a two-sample distance-correlation test [24], [25] between the original and bootstrap graphs: a large p-value suggests that the resampled graph has the same distribution as the original graph, while a small p-value (say less than 0.05) implies the resampled graph is significantly different in distribution and thus breaking the intention of bootstrap.

Algorithm 3 Encoder Embedding for Graph Bootstrap

Require: A ∈ ℜⁿˣⁿ, Y ∈ {1, . . . , K}ⁿ, and resampling size n₂.
Ensure: Resampled adjacency matrix A₂ ∈ ℜⁿˣⁿ₂, corresponding label Y₂ ∈ {1, . . . , K}ⁿ₂, and a two-sample test p-value pval.

function GEE BOOTSTRAP(A, Y, n₂)
    [Z, W] = GEE(A, Y);
    ind = bootstrap(n, n₂);   // sampling n₂ indices with replacement from {1, . . . , n}
    Y₂ = Y[ind];              // resampled class labels
    Z₂ = Z[:, ind];           // resampled encoder embedding
    A₂ = zeros(n₂, n₂);
    for i = 1, . . . , n₂ do
        for j = i + 1, . . . , n₂ do
            A₂[i, j] = Bernoulli(Z₂[i, Y₂[j]]);
            A₂[j, i] = A₂[i, j];
        end for
    end for
    pval = twosample(Z, Z₂);
end function

Figure 7 visualizes the graph bootstrap results for the Political Blog and the Email Network (we pick these two graphs as they have clearer community structure and thus better for visualization). The resampled graph not only appears quantitatively similar to the original graph, but also yields a very large p-value from the two-sample test, suggesting the bootstrap graph is indiscernible from the original graph in distribution.

We repeat the bootstrap sampling at n₂ = 1000 for 1000 times, and compute the two-sample p-value for each replicate. Algorithm 3 yields a mean p-value of 0.75 for the political blog data. Moreover, only 0.4% of the replicates yields a p-value that is less than 0.05. In comparison, we also evaluated the naive bootstrap on graph adjacency: the mean p-value is 0.25, and 26% of the replicates have p-value less than 0.05. Therefore, adjacency encoder embedding offers a better solution for graph bootstrap.

8 CONCLUSION

In this paper we proposed the graph encoder embedding method. The theoretical soundness is proved via asymptotic convergence and normality, and the numerical advantages are demonstrated in classification, clustering, and bootstrap. Most importantly, the excellent numerical performance is achieved with a fraction of time vs existing methods, making the graph encoder embedding very attractive and uniquely poised for huge graph data.

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9 Proofs
Throughout the theorem proofs, without loss of generality we always assume:

- \( n_k = O(n) \);
- The class labels \( \{Y_j, j = 1, \ldots, n\} \) are fixed a priori.

The first assumption guarantees that each class is always non-trivial, which always holds when the class labels are being generated by a non-zero prior probability.

The second assumption assumes the class labels are fixed, or equivalently the proof is presented by conditioning on the class labels. This assumption facilitates the proof procedure and does not affect the results, because all asymptotic results hold regardless of the actual class labels, thus still true without conditioning. Since conditioning is the common first step throughout Theorem 1 to Theorem 4, we always assume fixed class labels in all proofs.

**Theorem 1.** Suppose \( A \sim \text{SBM}(B) \). For a given \( i \)-th vertex of class \( y \), its graph encoder embedding \( Z_i \) converges to the respective block probability vector:

\[
\|Z_i - B(:, y)\|_2 \xrightarrow{n \to \infty} 0.
\]

**Proof.** Under SBM, each dimension \( k = 1, \ldots, K \) of the vertex embedding satisfies

\[
Z_i^k = W^T(:, k)A(:, i) = \frac{\sum_{j=1}^n I(Y_j = k)A(j, i)}{n_k} = \frac{\sum_{j=1, j \neq i, Y_j = k} B(B(Y_j, y))}{n_k} = \frac{\sum_{j=1, j \neq i, Y_j = k} B(k, y)}{n_k}.
\]

If \( k = y \), the numerator is summation of \((n_k - 1)\) i.i.d. Bernoulli random variables (since the summation includes a diagonal entry of \( A \), which is always 0). Otherwise, we have \( k \neq y \) and a summation of \( n_k \) i.i.d. Bernoulli random variables.

As \( n \) increases, \( n_k = O(n) \to \infty \) for any \( k \). By law of large numbers it is immediate that

\[
Z_i^k \to B(k, y)
\]

dimension-wise. Concatenating every dimension of the embedding, we have

\[
\|Z_i - B(:, y)\|_2 \to 0.
\]

**Theorem 2.** Suppose \( A \sim \text{DC-SBM}(B, \{\theta_j\}) \). For a given \( i \)-th vertex of class \( y \), its graph encoder embedding \( Z_i \) converges to the block probability vector up-to the degree coefficients:

\[
\|Z_i - \theta_i \cdot B(:, y) \odot \bar{\Theta}\|_2 \xrightarrow{n \to \infty} 0,
\]

where \( \bar{\Theta} = [\bar{\theta}_{(1)}, \cdots, \bar{\theta}_{(K)}] \in \mathbb{R}^K \) and \( \bar{\theta}_{(k)} = E(\theta_j | Y_j = k) \) denotes the class-conditional mean of vertex degrees, and \( \odot \) denotes the entry-wise multiplication.

**Proof.** Under DC-SBM, we have

\[
Z_i^k = W^T(:, k)A(:, i) = \frac{\sum_{j=1, j \neq i, Y_j = k} A(j, i)}{n_k} = \frac{\sum_{j=1, j \neq i, Y_j = k} \theta_j \theta_i B(k, y)}{n_k}.
\]

The numerator in second line is a summation of either \( n_k \) or \((n_k - 1)\) independent Bernoulli random variables. Without loss of generality, we shall assume \( k \neq y \) and \( n_k \) summands in the third line, which is asymptotically equivalent.

Note that given vertex \( i \), \( \theta_i \) and \( B(k, y) \) are fixed constants; and unlike the case of SBM, each random variable is now weighted by the degree coefficient and thus not identical. Since all degree coefficients lie in \((0, M]\), we have

\[
Var(Z_i^k) \leq \frac{\theta_i^2 M^2 \sum_{j=1, j \neq i, Y_j = k} B(k, y)(1 - B(k, y))}{n_k^2} \leq \frac{\theta_i^2 M^2}{4n_k}.
\]

As \( n \to \infty \) and \( n_k = O(n) \), \( Var(Z_i^k) \to 0 \) for each dimension \( k \).
By Chebychev inequality, $Z^k_i$ shall converge to its mean, which equals

\[
E(Z^k_i) = E\left(\frac{\sum_{j=1,j\neq i}^n I(Y_j = k)\theta_j \theta_i B(k, y)}{n_k}\right)
= \frac{\sum_{j=1,j\neq i}^n I(Y_j = k) E(\theta_j) E(Bern(B(k, y)))}{n_k}
= \frac{\theta_i B(k, y) \sum_{j=1,j\neq i}^n I(Y_j = k) E(\theta_j | Y_j = k)}{n_k}
= \theta_i B(k, y) \bar{\theta}(k).
\]

Concatenating every dimension of the embedding, it follows that

\[
\|Z_i - \theta_i B(:, y) \odot \bar{\Theta}\|_2 \to 0.
\]

\[\square\]

**Theorem 3.** Suppose $A \sim \text{RDPG}(\{X_i\})$. For a given $i$th vertex with an associated latent position $x_i \in \mathbb{R}^p$, its graph encoder embedding $Z_i$ converges to the latent position multiplied by the class-conditional means:

\[
\|Z_i - \lambda^T x_i\|_2 \overset{n \to \infty}{\to} 0,
\]

where $\lambda = [\lambda_1, \lambda_2, \ldots, \lambda_K] \in \mathbb{R}^{p \times K}$ and $\lambda_k = E(X | Y = k) \in \mathbb{R}^p$ denotes the class-conditional mean of the latent variable.

**Proof.** Under RDPG, we have

\[
Z^k_i = W^T(:, k) A(:, i)
= \frac{\sum_{j=1,j\neq i}^n A(j, i) I(Y_j = k) B(k, y)}{n_k}
= \frac{\sum_{j=1,j\neq i}^n Bern(X^T_j x_i)}{n_k},
\]

and it suffices to assume $k \neq y$ and thus $n_k$ summands in the third line. Note that given vertex $i$ and its latent position, the randomness only comes from $X_j$ and Bernoulli.

The expectation satisfies

\[
E(Z^k_i) = E\left(\frac{\sum_{j=1,j\neq i}^n I(Y_j = k) Bern(X^T_j x_i)}{n_k}\right)
= \frac{\sum_{j=1,j\neq i}^n I(Y_j = k) E(Bern(X^T_j x_i))}{n_k}
= \frac{\sum_{j=1,j\neq i}^n I(Y_j = k) E(E(Bern(X^T_j x_i) | X_j))}{n_k}
= \frac{\sum_{j=1,j\neq i}^n I(Y_j = k) E(X^T_j x_i)}{n_k}
= \frac{\sum_{j=1,j\neq i}^n I(Y_j = k) x_i}{n_k}
= \lambda^T_k x_i.
\]
And the variance satisfies
\[
\text{Var}(Z^k) = \sum_{j=1, j \neq i, Y_j = k}^n \frac{\text{Var}(\text{Bern}(X^T_j x_i))}{n_k^2} = \sum_{j=1, j \neq i, Y_j = k}^n \frac{\text{Var}(E(\text{Bern}(X^T_j x_i) | X_j)) + E(\text{Var}(\text{Bern}(X^T_j x_i) | X_j))}{n_k^2} = \sum_{j=1, j \neq i, Y_j = k}^n \frac{\text{Var}(X^T_j x_i) + E((X^T_j x_i)(1 - X^T_j x_i))}{n_k^2} = \sum_{j=1, j \neq i, Y_j = k}^n \frac{E((X^T_j x_i)^2) - E^2(X^T_j x_i) + E(X^T_j x_i) - E((X^T_j x_i)^2)}{n_k^2} = \sum_{j=1, j \neq i, Y_j = k}^n \frac{E(X^T_j x_i) - E^2(X^T_j x_i)}{n_k^2} \leq \frac{1}{4n_k}.
\]

As \(n_k = O(n)\) and the numerator is bounded in \([0, \frac{1}{4}]\) (due to the valid probability constraint in RDPG), the variance converges to 0 as sample size increases. Then by Chebychev inequality, \(Z^k_i \rightarrow \lambda^k x_i\). Concatenating every dimension of the embedding, it follows that
\[
\|Z_i - \lambda^T x_i\|_2 \rightarrow 0.
\]

\[\Box\]

**Theorem 4.** The graph encoder embedding is asymptotically normally distributed under SBM, DC-SBM, or RDPG. Specifically, as sample size increases, for a given \(i\)th vertex we have

- under SBM Graph:
  \(\text{Diag}(\bar{n})^{0.5} \cdot (Z_i - B(:, y)) \xrightarrow{d} N(0, \Sigma_B(:, y))\);
- under DC-SBM Graph:
  \(\text{Diag}(\bar{n})^{0.5} \cdot (Z_i - \theta_i B(:, y) \otimes \bar{\Theta}) \xrightarrow{d} N(0, \theta_i^2 \text{Diag}(\bar{\Theta}^2) \cdot \Sigma_B(:, y))\);
- under RDPG Graph:
  \(\text{Diag}(\bar{n})^{0.5} \cdot (Z_i - \lambda^T x_i) \xrightarrow{d} N(0, \text{Diag}(\lambda^T x_i - \bar{\lambda}^2(x_i)))\).

**Proof.** (i. SBM):
From proof of Theorem 1, it suffices to assume \(k \neq y\) and
\[
Z^k_i = \frac{\sum_{j=1, j \neq i, Y_j = k}^n \text{Bern}(B(k, y))}{n_k}.
\]
Applying central limit theorem to each dimension, we immediately have
\[
\sqrt{n_k}(Z^k_i - B(k, y)) \xrightarrow{d} N(0, B(k, y)(1 - B(k, y))).
\]
Note that \(Z^k_i\) and \(Z^l_i\) are always independent when \(k \neq l\). This is because every vertex belongs to a unique class, so the same Bernoulli random variable never appears in another dimension. Concatenating every dimension yields
\[
\text{Diag}(\bar{n})^{0.5} \cdot (Z_i - B(:, y)) \xrightarrow{d} N(0, \Sigma_B).
\]

(ii. DC-SBM):
From proof of Theorem 2, we have
\[
Z^k_i = \frac{\sum_{j=1, j \neq i, Y_j = k}^n \theta_i \theta_j \text{Bern}(B(k, y))}{n_k}.
\]
Namely, each dimension of the encoder embedding is a summation of \(n_k\) independent and weighted Bernoulli random variables that are no longer identical.

Omitting the scalar constant \(\theta_i\) in every summand, it suffices to check the Lyapunov condition for \(\{W_j = \theta_j \text{Bern}(B(k, y))\}\). Namely, prove that
\[
\lim_{n \to \infty} \frac{1}{s_n^3} \sum_{j=1}^{n_k} E(|W_j - E(W_j)|^3) = 0
\]
where \( s^2_{nk} \) is the summation of variances of \( \{W_j\} \). Based on the variance computation in the proof of Theorem 2, and note that all degree coefficients \( \theta_j \) are bounded in \((0, M]\), we have

\[
s^2_{nk} = \sum_{j=1, j \neq i}^{n} \text{Var}(\theta_j | Y_j = k)I(Y_j = k)B(k, y)(1 - B(k, y)) = O(n_k),
\]

\[
\sum_{j=1}^{n_k} E(|W_j - E(W_j)|^3) = \sum_{j=1, j \neq i}^{n} E(\theta_j^3 | Y_j = k)I(Y_j = k)E[Bern(B(k, y)) - B(k, y)]^3 = O(n_k).
\]

It follows that

\[
\frac{1}{n^3_k} \sum_{j=1}^{n_k} E(|W_j - E(W_j)|^3) = O(\frac{1}{\sqrt{n_k}}) \to 0,
\]

so the Lyapunov condition is satisfied.

Using Lyapunov central limit theorem and basic algebraic manipulation, we have

\[
\sqrt{n_k}(Z^k_i - \theta_i B(k, y)\bar{\theta}(k)) \xrightarrow{d} \mathcal{N}(0, \theta_i^2 \bar{\theta}(k)^2 B(k, y)(1 - B(k, y))).
\]

Concatenating every dimension yields

\[
\text{Diag}(\bar{\mu})^{0.5} \cdot (Z_i - \theta_i B(;, y) \otimes \Theta) \xrightarrow{d} \mathcal{N}(0, \theta_i^2 \text{Diag}(\bar{\theta}^2) \cdot \Sigma_B).
\]

(iii. RDPG):

From proof of Theorem 3,

\[
Z^k_i = \sum_{j=1, j \neq i}^{n_k} \text{Bern}(X^T_j x_i)
\]

which is a summation of \( n_k \) independent Bernoulli random variables.

Next we check the Lyapunov condition for \( \{W_j = \text{Bern}(X^T_j x_i)\} \):

\[
s^2_{nk} = \sum_{j=1, j \neq i}^{n} I(Y_j = k)\text{Var}(\text{Bern}(X^T_j x_i)) = O(n_k),
\]

\[
\sum_{j=1}^{n_k} E(|W_j - E(W_j)|^3) = \sum_{j=1, j \neq i}^{n} I(Y_j = k)E[\text{Bern}(X^T_j x_i) - E(X^T_j x_i)]^3 = O(n_k).
\]

This is because the variance and the third moments are all bounded, due to the Bernoulli random variable and \( X^T_j x_i \) being always bounded in \((0, 1]\). It follows that

\[
\frac{1}{n^3_k} \sum_{j=1}^{n_k} E(|W_j - E(W_j)|^3) = O(\frac{1}{\sqrt{n_k}}) \to 0,
\]

so the Lyapunov condition is satisfied.

Next, from proof of Theorem 3, we have

\[
\text{Var}(Z^k_i) = \sum_{j=1, j \neq i}^{n} E(X^T_j x_i) - E^2(X^T_j x_i) \sum_{j=1}^{n_k} \frac{E(X^T_j I(Y_j = k)x_i) - E^2(X^T_j I(Y_j = k)x_i)}{n_k^2} = \frac{\lambda^T_k x_i}{n_k} - \sum_{j=1, j \neq i}^{n} \frac{E^2(X^T_j I(Y_j = k)x_i)}{n_k^2}.
\]

Then by the Lyapunov central limit theorem, we have

\[
\sqrt{n_k}(Z^k_i - \lambda^T_k x_i) \xrightarrow{d} \mathcal{N}(0, \lambda^T_k x_i - \lambda^T_k x_i^2).
\]

Concatenating every dimension yields

\[
\text{Diag}(\bar{\mu})^{0.5} \cdot (Z_i - \lambda^T_k x_i) \xrightarrow{d} \mathcal{N}(0, \text{Diag}(\lambda^T x_i - \lambda^T k x_i^2)).
\]

\[\square\]
\section{Simulation Details}

\subsection{Figure 1}
For each model in Figure 1, we always set $Y_i = 1, 2$ with probability 0.5 and 0.5. Sample size is $n = 2000$.
For the SBM graph, the block probability matrix is set to
\[ B = \begin{bmatrix} 0.13, 0.1 \\ 0.1, 0.13 \end{bmatrix}. \]
For DC-SBM, we set the block probability matrix as
\[ B = \begin{bmatrix} 0.9, 0.1 \\ 0.1, 0.5 \end{bmatrix}, \]
then set $\theta_i \sim \text{Beta}(1, 4)$ for each $i$.
For RDPG, we generate the latent variable $X$ via the Beta mixture:
\[ X_i \sim \begin{cases} \text{Beta}(1, 5) & \text{if } Y_i = 1; \\ \text{Beta}(5, 1) & \text{if } Y_i = 2. \end{cases} \]

\subsection{Figure 2}
We set $Y_i = 1, 2$ with probability 0.5 and 0.5. Then for the SBM graphs in Figure 2, we set $n = 3000$ and the block probability matrix as
\[ B = \begin{bmatrix} 0.2, 0.1 \\ 0.1, 0.1 \end{bmatrix} \]
for graph 1.
For graph 2, we set
\[ B = \begin{bmatrix} 0.1, 0.2 \\ 0.2, 0.1 \end{bmatrix}. \]
For graph 3, we set
\[ B = \begin{bmatrix} 0.1, 0.2 \\ 0.2, 0.4 \end{bmatrix}. \]
For the DC-SBM models in Figure 2, we use the same block probability in each corresponding row, use $n = 5000$, and generate $\theta_i \sim \text{Uniform}(0.1, 0.5)$.
For RDPG, we set $n = 3000$ and generate the latent variable $X$ via the Beta mixture:
\[ X_i \sim \begin{cases} \text{Beta}(2, 3) & \text{if } Y_i = 1; \\ \text{Beta}(3, 2) & \text{if } Y_i = 2. \end{cases} \]
for graph 1.
For graph 2, we let
\[ X_i \sim \begin{cases} \text{Uniform}(0.15, 0.25) & \text{if } Y_i = 1; \\ \text{Uniform}(0.1, 0.2) & \text{if } Y_i = 2. \end{cases} \]
For graph 3, we let
\[ X_i \sim \begin{cases} \text{Normal}(0.15, 0.01) & \text{if } Y_i = 1; \\ \text{Normal}(0.2, 0.03) & \text{if } Y_i = 2. \end{cases} \]

\subsection{Classification Simulations in Figure 4}
For each model, we always set $Y_i = 1, 2, 3$ with probability 0.2, 0.3, 0.5 respectively.
For the SBM graph, the block probability matrix is
\[ B = \begin{bmatrix} 0.13, 0.1, 0.1 \\ 0.1, 0.13, 0.1 \\ 0.1, 0.1, 0.13 \end{bmatrix}. \]
For DC-SBM, we set the block probability matrix as
\[
B = \begin{bmatrix}
0.9, 0.1, 0.1 \\
0.1, 0.5, 0.1 \\
0.1, 0.1, 0.2 \\
\end{bmatrix},
\]
then set \( \theta_i \overset{i.i.d.}{\sim} \text{Beta}(1, 4) \) for each \( i \). For RDPG, we generate the latent variable \( X \) via the Beta mixture:
\[
X_i \overset{i.i.d.}{\sim} \begin{cases} 
\text{Beta}(1, 5) & \text{if } Y_i = 1; \\
\text{Beta}(5, 5) & \text{if } Y_i = 2; \\
\text{Beta}(5, 1) & \text{if } Y_i = 3.
\end{cases}
\]