Graph Encoder Embedding

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Manuscript: `https://arxiv.org/abs/2109.13098`

Code: `https://github.com/cshen6/GraphEmd`

Overview

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2. Graph Encoder Embedding
3. Running Time Advantage
4. Theoretical Properties
5. Vertex Classification
6. Vertex Clustering

Section 1

Introduction

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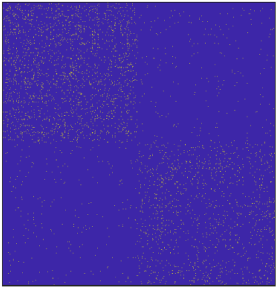
In practice, a graph is typically stored by an $s \times 3$ edgelist $\mathbf{E}$, where the first two columns store the vertex indices of each edge and the last column is the edge weight.

Example

Adjacency Matrix Heatmap



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- Deepwalk / Node2vec : random-walk based method per vertex.
- Graph Convolutional Network : based on adjacency matrix and gradient descent.

Applications

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And many more graph-based questions: hypothesis testing, signal subgraph, outlier detection in graph time-series, hierarchical community detection, etc.

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We would like a scalable embedding method that is easy to implement, theoretically sound, numerically superior, and capable of processing billions of edges in minutes!

Section 2

Graph Encoder Embedding

Matrix Version with Partial Labels

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The ith row of $\mathbf{Z}$ represents the vertex embedding for vertex i, while the kth column represents the connectivity to class k. One may further normalize each row into norm 1.

Example

```
>> A

A =

     0     1     1     0     0
     1     0     1     0     0
     1     1     0     1     0
     0     0     1     0     1
     0     0     0     1     0

>> Y

Y =

     1
     1
     1
     2
     2
```

```
>> W=onehotencode(categorical(Y),2)

W =

     1     0
     1     0
     1     0
     0     1
     0     1

>> W(Y==1,1)=W(Y==1,1)/sum(Y==1)

W =

    0.3333         0
    0.3333         0
    0.3333         0
         0    1.0000
         0    1.0000
```

```
>> W(Y==2,2)=W(Y==2,2)/sum(Y==2)

W =

    0.3333         0
    0.3333         0
    0.3333         0
         0    0.5000
         0    0.5000

>> Z=A*W

Z =

    0.6667         0
    0.6667         0
    0.6667    0.5000
    0.3333    0.5000
         0    0.5000
```

The final embedding **Z** exhibits clear separation of community structure.

Edgelist Version

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The method is applicable to directed or weighted graphs, as well as graph Laplacian

$$\mathbf{Z} = \mathbf{D}^{-0.5}\mathbf{A}\mathbf{D}^{-0.5}\mathbf{W}.$$

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The time and storage complexity are $O(nk + s)$, i.e., linear with respect to the number of vertices and number of edges.

Section 3

Running Time Advantage

In the next figure we plot the average running time of graph encoder embedding using 50 Monte Carlo replicates, on a random graph with $K = 10$, average degree 100, and increasing graph size.

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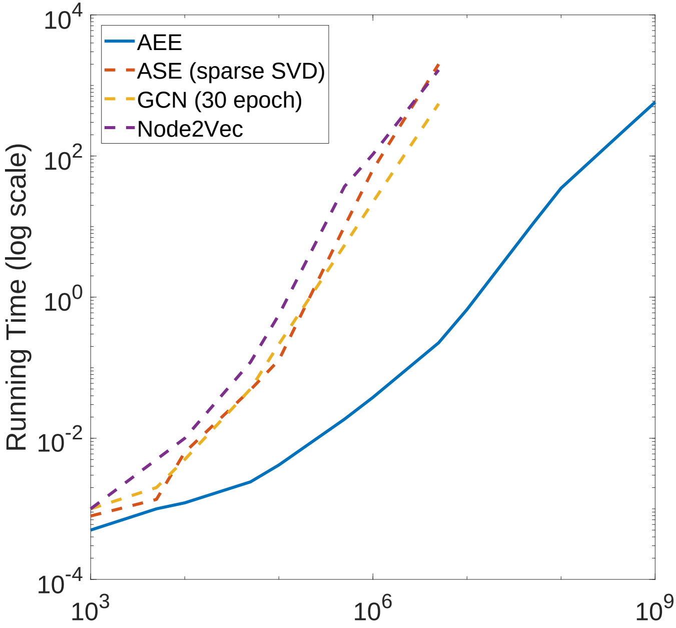
The number of edges increases from one thousand to one billion. At 1 billion edges with 10 million vertices, the encoder embedding only requires 20GB memory and finishes in 10 minutes. All other methods exceed maximum memory capacity at 10 million edges.



AEE
ASE (sparse SVD)
GCN (30 epoch)
Node2Vec
Running Time (log scale)
10^4
10^2
10^0
10^{-2}
10^{-4}
10^3
10^6
10^9

To validate the running time, we conducted extensive time comparison among various implementations of spectral embedding and node2vec on MATLAB, R, and Python.

[1] https://github.com/microsoft/graspologic/

[2] https://github.com/aditya-grover/node2vec

[3] https://https://github.com/eliorc/node2vec

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For node2vec, we compared various implementations from original authors' C and Python code[2], another Python implementation[3], R version, Python code from Microsoft, and PecanPy[4].

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Section 4

Theoretical Properties

Stochastic Block Model

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

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Then a block probability matrix $\mathbf{B} = [\mathbf{B}(k,l)] \in [0,1]^{K \times K}$ specifies the edge probability between a vertex from class k and a vertex from class l: for any $i < j$,

$$\mathbf{A}(i,j) \overset{i.i.d.}{\sim} \text{Bernoulli}(\mathbf{B}(Y_i, Y_j)),$$
$$\mathbf{A}(i,i) = 0, \quad \mathbf{A}(j,i) = \mathbf{A}(i,j).$$

Degree-Corrected SBM

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The degree parameters typically require certain constraint to ensure a valid probability. In this paper we simply assume they are non-trivial and bounded, i.e., $\theta_i \overset{i.i.d.}{\sim} F_\theta \in (0, M]$, which is a very general assumption.

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To generate communities under RDPG, it suffices to use a K-component mixture distribution, i.e., let $(X_i, Y_i) \stackrel{i.i.d.}{\sim} F_{XY}$ be a distribution on $\mathbb{R}^p \times [K]$.

Central Limit Theorem

Theorem 1

The graph encoder embedding is asymptotically normally distributed under SBM, DC-SBM, or RDPG. Specifically, as n increases, for a given ith vertex of class y it holds that

$$Diag(\vec{n})^{0.5} \cdot (\mathbf{Z}_i - \mu) \xrightarrow{d} \mathcal{N}(0, \Sigma),$$

where $\vec{n} = [n_1, n_2, \cdots, n_k] \in \mathbb{R}^K$*, and* $Diag(\cdot)$ *is the diagonal matrix of a vector.*

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where $\vec{n} = [n_1, n_2, \cdots, n_k] \in \mathbb{R}^K$*, and* $Diag(\cdot)$ *is the diagonal matrix of a vector. The expectation and covariance are:*

- *under SBM,* $\mu = \mathbf{B}(:, y)$ *and* $\Sigma = \Sigma_{\mathbf{B}(:,y)}$*;*
- *under DC-SBM,* $\mu = \theta_i \mathbf{B}(:, y) \odot \bar{\Theta}^{(1)}$ *and* $\Sigma = \theta_i^2 Diag(\bar{\Theta}^{(2)}) \cdot \Sigma_{\mathbf{B}(:,y)}$*;*
- *under RDPG,* $\mu = \bar{\lambda}_{X_i}^{(1)}$ *and* $\Sigma = Diag(\bar{\lambda}_{X_i}^{(1)} - \bar{\lambda}_{X_i}^{(2)})$*.*

Central Limit Theorem

- Under SBM with block matrix $\mathbf{B}$, define $\Sigma_{\mathbf{B}(:,y)}$ as the $K \times K$ diagonal matrix with

$$\Sigma_{\mathbf{B}(:,y)}(k,k) = \mathbf{B}(k,y)(1 - \mathbf{B}(k,y)) \in [0, \frac{1}{4}].$$

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- Under DC-SBM with $\{\theta_j \overset{i.i.d.}{\sim} F_\theta\}$, for any tth moment we define:

$$\bar{\theta}_k^{(t)} = E(\theta_j^t | Y_j = k),$$
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- Under RDPG where $(X, Y) \sim F_{XY} \in \mathbb{R}^p \times [K]$ is the latent distribution, define

$$\begin{aligned} \bar{\lambda}_k^{(t)}(x_i) &= E^t(X^T x_i | Y = k), \\ \bar{\lambda}_{x_i}^{(t)} &= [\bar{\lambda}_1^{(t)}(x_i), \bar{\lambda}_2^{(t)}(x_i), \cdots, \bar{\lambda}_K^{(t)}(x_i)] \in \mathbb{R}^K \end{aligned}$$

for any fixed vector $x_i \in \mathbb{R}^p$.

Law of Large Numbers

Corollary 1 (Consistency)

Using the same notation as in Theorem 1. It always holds that

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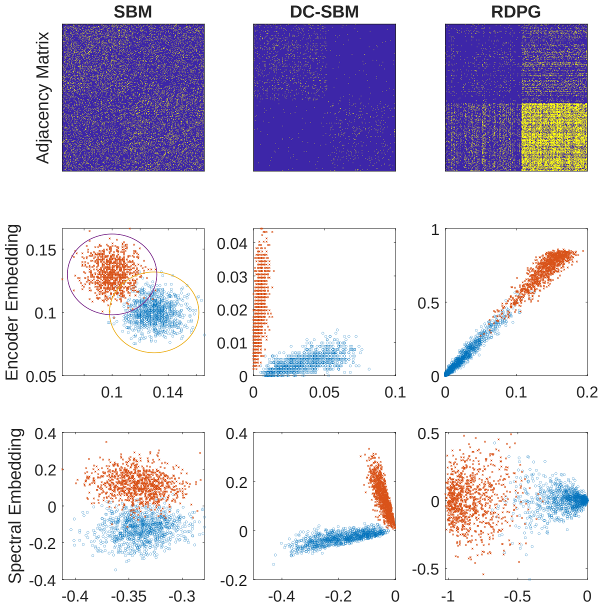
The asymptotic normality and asymptotic convergence also hold for weighted graphs.

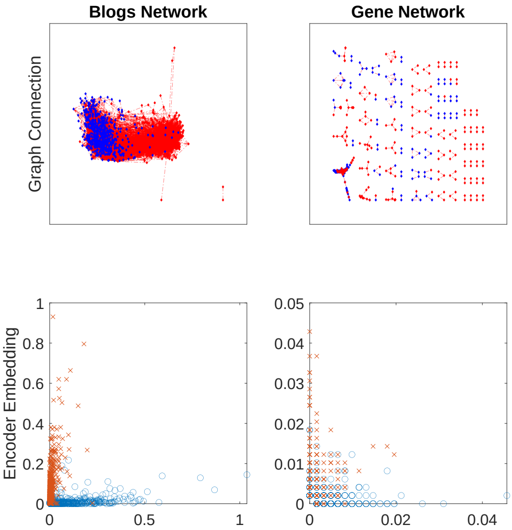
Visualization

We first compare the graph encoder embedding to the spectral embedding under SBM, DC-SBM, and RDPG graphs at $K = 2$. While both methods exhibit clear community separation, the encoder embedding provides better estimation for the model parameters.


SBM
DC-SBM
RDPG
Adjacency Matrix
Encoder Embedding
Spectral Embedding
0.15
0.1
0.05
0.1
0.14
0.04
0.03
0.02
0.01
0
0
0.05
0.1
1
0.5
0
0
0.1
0.2
0.4
0.2
0
-0.2
-0.4
-0.4
-0.35
-0.3
0.4
0.2
0
-0.2
-0.4
-0.2
0
0.5
0
-0.5
-1
-0.5
0

Visualization

Then we inspect graph encoder embedding for the Political Blogs (1490 vertices with 2 classes) and the Gene Network (1103 vertices with 2 classes). Both graphs are sparse. The average degree is 22.4 for the Political Blogs and 1.5 for the Gene Network.


Blogs Network
Gene Network
Graph Connection
Encoder Embedding
1
0.8
0.6
0.4
0.2
0
0.5
1
0.05
0.04
0.03
0.02
0.01
0
0.02
0.04

Section 5

Vertex Classification

Simulated Data

An immediate and important use case herein is vertex classification. The vertex embedding with known class labels are the training data (labels with class 1 to K), while the vertex embedding with unknown labels are the testing data (labels set to 0 in the method).

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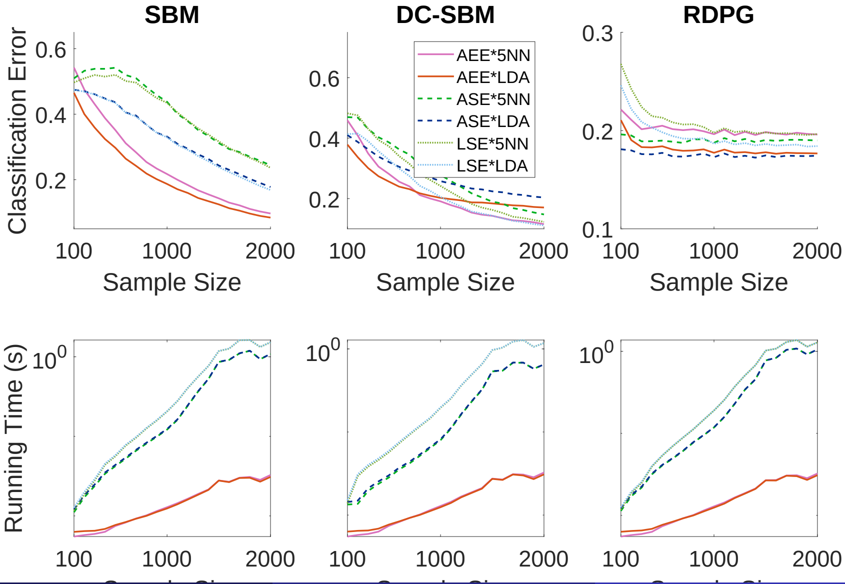
For every embedding, we use linear discriminant analysis (LDA) and 5-nearest-neighbor (5NN) as the follow-on classifiers. Other classifier like logistic regression, random forest, and neural network can also be used. We observe similar accuracy regardless of the classifiers, implying that the learning task largely depends on the embedding method.

Simulated Data



Real Data

We downloaded a variety of public real graphs with labels, including three graphs from network repository[5]:

- Cora Citations (2708 vertices, 5429 edges, 7 classes),
- Gene Network (1103 vertices, 1672 edges, 2 classes),
- Industry Partnerships (219 vertices, 630 edges, 3 classes);

and three more graphs from Stanford network data[6]:

- EU Email Network (1005 vertices, 25571 edges, 42 classes),
- LastFM Asia Social Network (7624 vertices, 27806 edges, 17 classes),
- Political Blogs (1490 vertices, 33433 edges, 2 classes).

[5] http://networkrepository.com/

[6] https://snap.stanford.edu/

Classification Error

	AEE	LEE	ASE	LSE	N2v	Chance
Cora	16.3%	**15.5%**	31.0%	33.1%	16.3%	69.8%
Email	30.6%	28.3%	30.8%	39.5%	**26.1%**	89.2%
Gene	17.1%	**16.5%**	27.2%	36.2%	21.9%	44.4%
Industry	**29.7%**	30.7%	38.8%	39.2%	32.9%	39.3%
LastFM	15.5%	15.0%	20.1%	16.5%	**14.5%**	79.4%
PolBlog	4.9%	5.0%	5.5%	**4.0%**	4.5%	48.0%

Running Time (seconds)

	AEE	LEE	ASE	LSE	N2v	
Cora	**0.01**	**0.01**	1.55	1.60	2.1	
Email	**0.02**	0.03	0.12	0.15	1.2	
Gene	**0.01**	**0.01**	0.15	0.18	0.80	
Industry	**0.01**	**0.01**	0.02	0.02	0.25	
LastFM	**0.02**	0.03	13.0	15.3	9.2	
PolBlog	**0.01**	0.02	0.27	0.28	1.2	

Section 6

Vertex Clustering

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The algorithm stops when the labels no longer change or the maximum iteration limit is reached.

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- **Step 4**: If $ARI(\mathbf{Y}, \mathbf{Y}_2) = 1$ or max iteration reached, stop the algorithm. Otherwise set $\mathbf{Y}_2 = \mathbf{Y}$ and repeat from Step 2.
- **Output**: The final embedding $\mathbf{Z} \in \mathbb{R}^{n \times K}$, and final label vector $\mathbf{Y}$.

This is both an embedding and clustering algorithm. The running time is $O(M(nK^2 + s))$, which is still linear with respect to the number of edges and the number of vertices.

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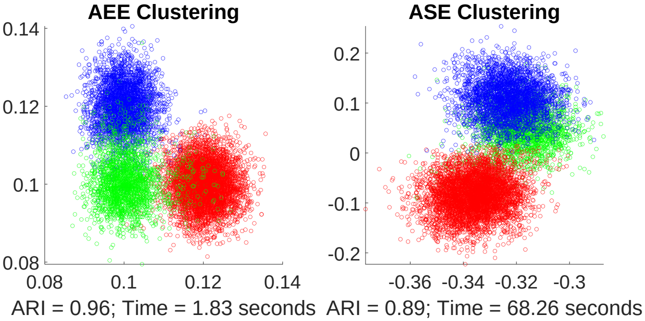
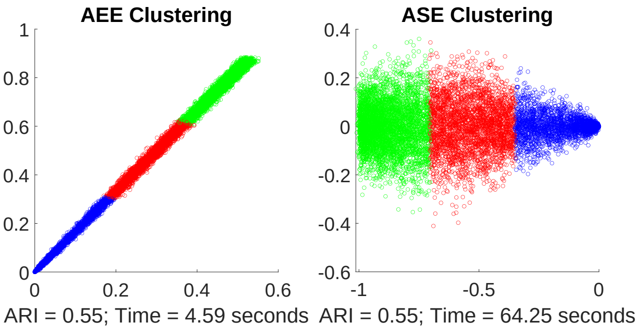
Instead of a determined K, we have enhanced the algorithm to work for a range of K then pick the best possible group based on certain metric. Moreover, to guard against possible bad initialization, the algorithm also has a parameter to re-do initialization.

SBM Simulation



RDPG Simulation



Clustering ARI on Same Real Graphs

	AEE	LEE	ASE	LSE	N2v
Cora	0.12	0.07	0.08	0.01	**0.24**
Email	**0.40**	0.39	0.11	0.21	0.34
Gene	0.01	0.01	0.01	0.01	0.00
Industry	**0.13**	0.03	0.01	0.02	**0.13**
LastFM	0.34	0.19	0.03	**0.47**	0.43
PolBlog	**0.80**	0.58	0.07	**0.80**	**0.80**

Running Time (seconds)

	AEE	LEE	ASE	LSE	N2v
Cora	**0.11**	0.12	1.6	1.7	2.2
Email	0.18	0.28	**0.13**	0.20	1.3
Gene	**0.03**	**0.03**	0.17	0.20	0.90
Industry	0.02	0.02	0.02	0.02	0.40
LastFM	**0.35**	0.39	13.6	15.5	9.5
PolBlog	**0.05**	0.07	0.27	0.29	1.4

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4. Excellent numerical performance: achieved excellent performance in classification error and clustering ARI throughout synthetic and real data experiments. The performance is on par with existing approaches but much faster.