Bias-Variance Tradeoffs in Joint Spectral Embeddings

Benjamin Draves Daniel Sussman

Boston University

Joint Statistical Meetings, 1 August 2019

Network Embeddings

- Goal: Represent vertices of a network in a low dimensional space
- Reason: Use machine learning techniques to answer network based questions



Analysis Framework

- Consider m graphs over a common vertex set \mathcal{V} of size n
- Associate $v \in \mathcal{V}$ with a latent position $X_v \in \mathbb{R}^d$

Inner Product Distribution

Let *F* be a probability distribution over \mathbb{R}^d . We say *F* is a *d*-dimensional inner product distribution if all $\mathbf{x}, \mathbf{y} \in \text{supp}(F)$ has the property $\mathbf{x}^T \mathbf{y} \in [0, 1]$.

Assume latent positions X₁, X₂,..., X_n ^{i.i.d.} ∼ F. Organize in the rows of a matrix X = [X₁X₂...X_n]^T.

Technical Assumption

For $\mathbf{y} \sim F$ assume $\Delta = \mathbb{E}[\mathbf{y}\mathbf{y}^T]$ is diagonal with $\min_{i \in [d]} \Delta_{ii} > 0$

Multiplex Colinear Random Dot Product Graph

Multiplex Colinear Random Dot Product Graph (MCRDPG)

- Let $\mathbf{C}^{(1)}, \ldots, \mathbf{C}^{(m)} \in \mathbb{R}^{d \times d}$ be a diagonal matrices with non-negative entries so that $\mathbf{X}_i^T \mathbf{C}^{(g)} \mathbf{X}_j \in [0, 1]$ for all $i \in [n]$ and $g \in [m]$.
- The random adjacency matrices $\{\mathbf{A}^{(g)}\}_{g=1}^{m}$ are distributed according to the *MCRDPG* with *latent positions* **X** iff $\{\mathbf{A}_{ij}^{(g)}\}$ are conditionally independent with

$$\mathbb{P}(\mathbf{A}_{ij}^{(g)} = 1 | \mathbf{X}) = \mathbf{X}_i^T \mathbf{C}^{(g)} \mathbf{X}_j$$

- In essence, $\mathbf{A}_{ij}^{(g)} | \mathbf{X} \stackrel{ind.}{\sim} \operatorname{Bern}(\mathbf{X}_i^T \mathbf{C}^{(g)} \mathbf{X}_j)$
- Task: Given $\{\mathbf{A}^{(g)}\}_{g=1}^{m}$, how do we estimate $\{\mathbf{X}\sqrt{\mathbf{C}^{(g)}}\}_{g=1}^{m}$?

Adjacency Spectral Embedding

• Idea 1: Ignore joint structure and estimate $X\sqrt{C^{(g)}}$ individually

Adjacency Spectral Embedding (Sussman et al. 2012)

Let $\mathbf{A}^{(g)}$ have eigendecomposition

$$\mathbf{A}^{(g)} = [\mathbf{U}_{\mathbf{A}^{(g)}} | \tilde{\mathbf{U}}_{\mathbf{A}^{(g)}}] [\mathbf{S}_{\mathbf{A}^{(g)}} \oplus \tilde{\mathbf{S}}_{\mathbf{A}^{(g)}}] [\mathbf{U}_{\mathbf{A}^{(g)}} | \tilde{\mathbf{U}}_{\mathbf{A}^{(g)}}]^T$$

where $\mathbf{U}_{\mathbf{A}^{(g)}} \in \mathbb{R}^{n \times d}$ and $\mathbf{S}_{\mathbf{A}^{(g)}} \in \mathbb{R}^{d \times d}$ contains the top d eigenvalues of $\mathbf{A}^{(g)}$. Then the ASE of $\mathbf{A}^{(g)}$ is defined by $ASE(\mathbf{A}^{(g)}, d) = \mathbf{U}_{\mathbf{A}^{(g)}} \mathbf{S}_{\mathbf{A}^{(g)}}^{1/2}$.

- Estimate $\mathbf{X}\sqrt{\mathbf{C}^{(g)}}$ by $\hat{\mathbf{X}}_{ASE}^{(g)} = ASE(\mathbf{A}^{(g)}, d)$
- Idea 2: Assume i.i.d. $(\mathbf{C}^{(g)} = \mathbf{C}^*)$ and estimate a global $\hat{\mathbf{X}}$
- Estimate $X\sqrt{C^{(g)}}$ by $\hat{X}_{Abar} = ASE(\bar{A}, d)$ where $\bar{A} = m^{-1}\sum_{g=1}^{m} A^{(g)}$

Omnibus Embedding

• Idea 3: Incorporate the joint structure in the embedding

Omnibus Embedding (Levin et al. 2017)

The Omnibus matrix is given by

$$\tilde{\mathbf{A}} = \begin{bmatrix} \mathbf{A}^{(1)} & \frac{1}{2} [\mathbf{A}^{(1)} + \mathbf{A}^{(2)}] & \dots & \frac{1}{2} [\mathbf{A}^{(1)} + \mathbf{A}^{(m)}] \\ \frac{1}{2} [\mathbf{A}^{(2)} + \mathbf{A}^{(1)}] & \mathbf{A}^{(2)} & \dots & \frac{1}{2} [\mathbf{A}^{(2)} + \mathbf{A}^{(m)}] \\ \vdots & \vdots & \ddots & \vdots \\ \frac{1}{2} [\mathbf{A}^{(m)} + \mathbf{A}^{(1)}] & \frac{1}{2} [\mathbf{A}^{(m)} + \mathbf{A}^{(2)}] & \dots & \mathbf{A}^{(m)} \end{bmatrix}$$

- Notice $\mathsf{ASE}(\mathbf{\tilde{A}}, d) \in \mathbb{R}^{nm \times d}$
- Estimate $\mathbf{X}\sqrt{\mathbf{C}^{(g)}}$ by $\hat{\mathbf{X}}_{Omni}^{(g)} = [\mathsf{ASE}(\tilde{\mathbf{A}}, d)]_g$ where $[\cdot]_g$ denotes the g-th n row block.

Simulation: Mean Squared Error

- Suppose $\mathbf{A}^{(1)} \sim \mathsf{ER}(p)$ and $\mathbf{A}^{(2)} \sim \mathsf{ER}(c^2 p)$
- Then the latent positions are \sqrt{p} for ${f A}^{(1)}$ and $c\sqrt{p}$ for ${f A}^{(2)}$



Bias in Joint Spectral Embeddings

Preliminary notation:

• Let h = i + n(g - 1) for $i \in [n]$ and $g \in [m]$ and define $(\mathbf{M})_i = \mathbf{M}_{i}^T$

• Let
$$\mathbf{L} = [\sqrt{\mathbf{C}^{(1)}} \mathbf{X}^T \ \sqrt{\mathbf{C}^{(2)}} \mathbf{X}^T \dots \sqrt{\mathbf{C}^{(m)}} \mathbf{X}^T]^T$$

Theorem

- Let $(\{\mathbf{A}^{(g)}\}_{g=1}^m, \mathbf{X}) \sim MCRDPG(F, n, \{\mathbf{C}^{(g)}\}_{g=1}^m)$. Let $\hat{\mathbf{L}} = ASE(\tilde{\mathbf{A}}, d)$ be the Omnibus embedding of $\{\mathbf{A}^{(g)}\}_{g=1}^m$.
- There exists diagonal matrices {S^(g)}^m_{g=1} that only depend on {C^(g)}^m_{g=1} and an orthogonal matrix W such that

$$(\hat{\mathbf{L}}\mathbf{W} - \mathbf{L})_h = (\mathbf{S}^{(g)} - \sqrt{\mathbf{C}^{(g)}})\mathbf{X}_i + \mathbf{R}_h$$
(1)

Moreover, with high probability

$$\max_{m \in [nm]} \|\mathbf{R}_h\|_2 \le O\left(\frac{m^{3/2}\log nm}{\sqrt{n}}\right)$$
(2)

Benjamin Draves (Boston Univeristy)

Simulation Design

• Base model: Balanced two group SBM, $\mathbf{B} = \begin{bmatrix} 1/4 & 1/20\\ 1/20 & 1/4 \end{bmatrix}$

Network	Weighting	Block Probabilities	Model
A ⁽¹⁾	$\mathbf{C}^{(1)} = \begin{bmatrix} 3/4 & 0 \\ 0 & 1/2 \end{bmatrix}$	$\mathbf{B}_1 = \begin{bmatrix} 13/80 & 1/16 \\ 1/16 & 13/80 \end{bmatrix}$	Connected SBM
A ⁽²⁾	$\mathbf{C}^{(2)} = \begin{bmatrix} 1/2 & 0 \\ 0 & 3/4 \end{bmatrix}$	$\mathbf{B}_2 = \begin{bmatrix} 3/20 & 0 \\ 0 & 3/20 \end{bmatrix}$	Disconnected SBM
A ⁽³⁾	$\mathbf{C}^{(3)} = egin{bmatrix} 1 & 0 \ 0 & 0 \end{bmatrix}$	$\mathbf{B}_3 = \begin{bmatrix} 3/20 & 3/20 \\ \\ 3/20 & 3/20 \end{bmatrix}$	Erdös-Réyni

Simulation Design (continued)

Simulation Design

- **Q** Assign vertices to each group with probability $\pi = .5$
- ② Sample adjacency matrices

•
$$\mathbf{A}^{(2)} \sim \mathsf{SBM}(\mathbf{B}_2, \pi)$$

•
$$A^{(3)} \sim ER(p = 0.15)$$

- **3** Embed $\tilde{\mathbf{A}}$ to obtain $\hat{\mathbf{L}} = [\hat{\mathbf{X}}_{Omni}^{(1)T} \ \hat{\mathbf{X}}_{Omni}^{(2)T} \ \hat{\mathbf{X}}_{Omni}^{(3)T}]^T$
 - Compare analytic bias $(\mathbf{S}^{(g)} \sqrt{\mathbf{C}^{(g)}})\mathbf{X}_i$ to observed bias $(\hat{\mathbf{L}}\mathbf{W} \mathbf{L})_h$.
 - Compare residual bound $O\left(\frac{m^{3/2}\log nm}{\sqrt{n}}\right)$ to observed residuals $\hat{\mathbf{R}}_h$.

Simulation Results: Bias



Benjamin Draves (Boston Univeristy)

Simulation Results: Bias



Benjamin Draves (Boston Univeristy)

Simulation Results: Residuals



Benjamin Draves (Boston Univeristy)

Simulation Results: Residuals



Benjamin Draves (Boston Univeristy)

Variance in Joint Spectral Embeddings

Residual Decomposition

Decompose the residual term $\sqrt{n}\mathbf{R}_i = \sqrt{n}\mathbf{R}_i^{(1)} + \sqrt{n}\mathbf{R}_i^{(2)}$



Benjamin Draves (Boston Univeristy)

Variance in Joint Spectral Embeddings

Residual Decomposition

Decompose the residual term
$$\sqrt{n}\mathbf{R}_i = \sqrt{n}\mathbf{R}_i^{(1)} + \sqrt{n}\mathbf{R}_i^{(2)}$$



Benjamin Draves (Boston Univeristy)

Conclusion

- Introduced the MCRDPG probability model
- Highlighted an advantageous bias-variance tradeoff given by the Omnibus Embedding
- Established
 - Bias of the Omnibus Estimator under the MCRDPG
 - **2** Uniform bound on the residual term at a $O(m^{3/2} \log nm/\sqrt{n})$ rate
- Highlighted second moment properties of the Omnibus Embedding

Questions?

References I

- Avanti Athreya et al. "Statistical inference on random dot product graphs: A survey". In: *Journal of Machine Learning Research* 18 (Sept. 2017).
- A. Athreya et al. "A Limit Theorem for Scaled Eigenvectors of Random Dot Product Graphs". In: Sankhya A 78.1 (Feb. 2016), pp. 1–18.
- Peter D Hoff, Adrian E Raftery, and Mark S Handcock. "Latent Space Approaches to Social Network Analysis". In: *Journal of the American Statistical Association* 97.460 (2002), pp. 1090–1098.

Keith Levin et al. "A Central Limit Theorem for an Omnibus Embedding of Multiple Random Dot Product Graphs". In: Nov. 2017, pp. 964–967.

References II

- Daniel L. Sussman et al. "A Consistent Adjacency Spectral Embedding for Stochastic Blockmodel Graphs". In: Journal of the American Statistical Association 107.499 (2012), pp. 1119–1128.
- Shangsi Wang et al. Joint Embedding of Graphs. 2017.
- Stephen J. Young and Edward R. Scheinerman. "Random Dot Product Graph Models for Social Networks". In: Algorithms and Models for the Web-Graph. Ed. by Anthony Bonato and Fan R. K. Chung. Berlin, Heidelberg: Springer Berlin Heidelberg, 2007, pp. 138–149.