Structured Graph Learning via Laplacian Spectral Constraints

by

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Learning Undirected Graphs

State of the art:

$$
\begin{array}{ll}
\underset{\mathbf{\Theta}}{\text{maximize}} & \log \text{gdet}\, \mathbf{\Theta} - \operatorname{tr}(\mathbf{S}\mathbf{\Theta}) - \alpha \|\mathbf{\Theta}\|_{1,\text{off}}, \\
\text{subject to} & \mathbf{\Theta} \in \mathcal{S}_{\mathcal{L}},
\end{array} \tag{1}
$$

$$
\mathcal{S}_{\mathcal{L}} = \left\{ \mathbf{\Theta} \in \mathbb{R}^{p \times p} : \mathbf{\Theta}\mathbf{1} = \mathbf{0}, \mathbf{\Theta}_{ij} = \mathbf{\Theta}_{ji} \leq 0, \mathbf{\Theta} \succeq \mathbf{0} \right\}. \tag{2}
$$

- Existing methods fall short to impose prior knowledge of the graph structure
- Practical implications: the above framework can't handle multimodal graphs (e.g. k-component graphs)

Imposing Spectral Constraints

To overcome the shortcomings of the previous framework, we propose to constrain the eigenvalues of $\boldsymbol{\Theta}$:

$$\begin{array}{ll} \underset{\boldsymbol{\Theta}}{\text{maximize}} & \log \text{g}\det \boldsymbol{\Theta} - \mathrm{tr}(\mathbf{S}\boldsymbol{\Theta}) - \alpha\|\boldsymbol{\Theta}\|_{1,\text{off}}, \\ \text{subject to} & \boldsymbol{\Theta} \in \mathcal{S}_{\mathcal{L}}, \ \boldsymbol{\lambda}(\boldsymbol{\Theta}) \in \mathcal{S}_{\lambda}, \end{array} \tag{3}$$

- For k-component graph:
  $\mathcal{S}_\lambda = \{\{\lambda_i\}_{i=1}^{p} : \lambda_1 = \ldots = \lambda_k = 0,\ 0 < \lambda_{k+1} \leq \ldots \leq \lambda_p\}$
- Major issue: **NP-hard**.

Approximately Imposing Spectral Constraints

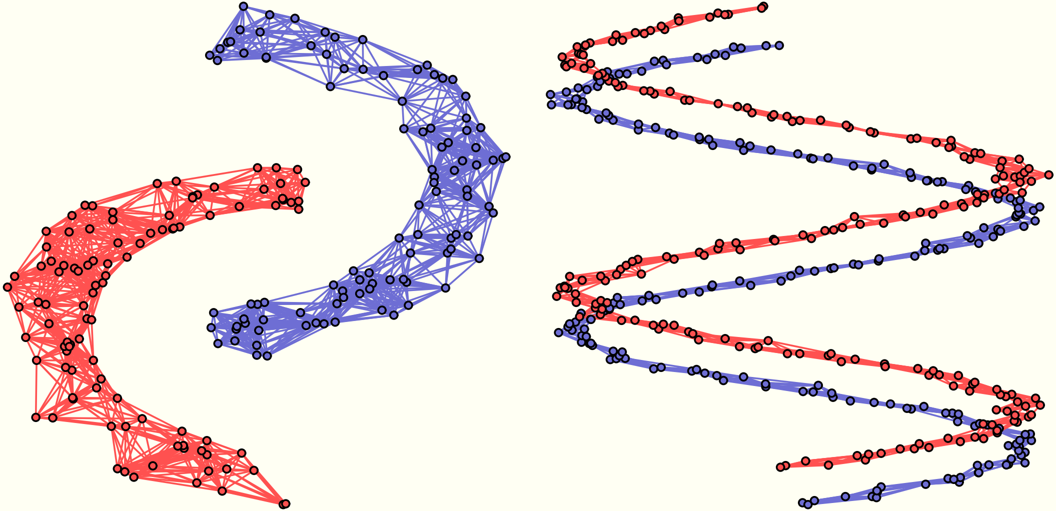
Approximating (3):

$$\begin{array}{ll}\underset{\mathbf{w},\boldsymbol{\lambda},\mathbf{U}}{\text{minimize}} & -\log \operatorname{gdet}\left(\operatorname{Diag}(\boldsymbol{\lambda})\right) + \operatorname{tr}\left(\mathbf{S}\mathcal{L}\mathbf{w}\right) + \alpha\|\mathcal{L}\mathbf{w}\|_1 + \frac{\beta}{2}\left\|\mathcal{L}\mathbf{w} - \mathbf{U}\operatorname{Diag}(\boldsymbol{\lambda})\mathbf{U}^T\right\|_F^2 \\ \text{subject to} & \mathbf{w} \geq 0, \boldsymbol{\lambda} \in \mathcal{S}_\lambda, \mathbf{U}^T\mathbf{U} = \mathbf{I}\end{array} \tag{4}$$

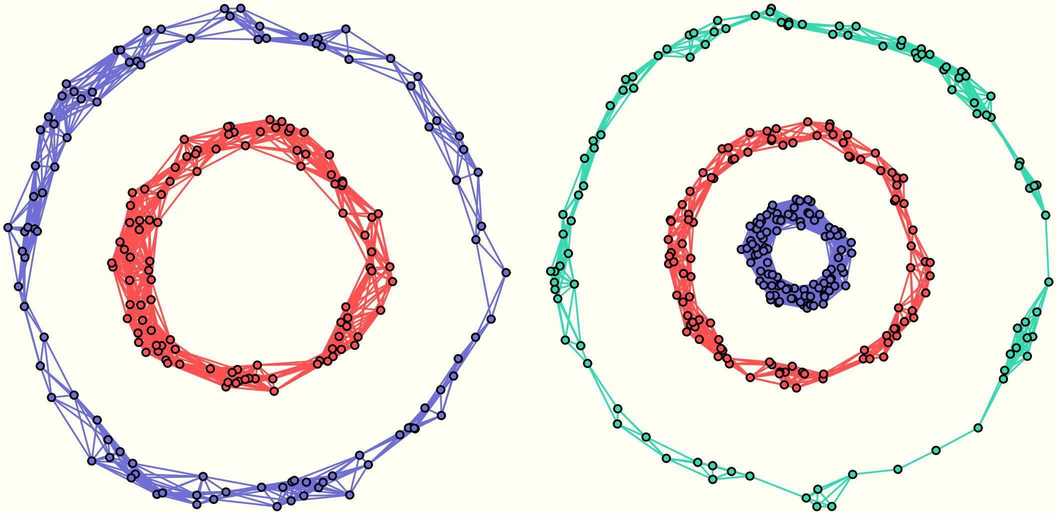
where $\mathcal{L}$ is a linear operator that maps a $p \times (p-1)$-vector into a valid $p \times p$ Laplacian matrix.

- Although still **non-convex**, we proposed a convergent, efficient algorithm based on the block successive upper-bound minimization (BSUM) method.

Sneak-peek on the results (toy data)

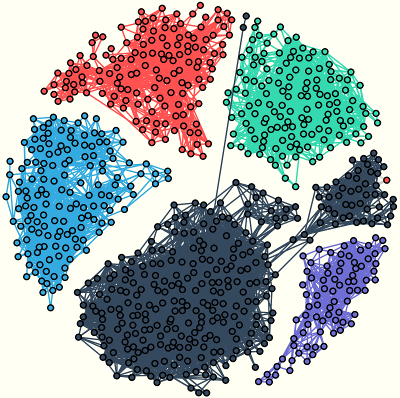


Sneak-peek on the results (toy data)



Sneak-peek on the results (real data)

- RNA-Seq Cancer Genome Atlas Research Network dataset:



Reproducibility

The code for the experiments can be found at

- `https://github.com/dppalomar/spectralGraphTopology`
- `https://cran.r-project.org/web/packages/spectralGraphTopology/`