

Representation Learning on Graphs and Networks (L45)

CST Part III / MPhil in ACS

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1 Primer on Graph Representations

1. Mathematical definition of graphs:

A graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ is a collection of nodes \mathcal{V} and edges $\mathcal{E} \subseteq \mathcal{V} \times \mathcal{V}$

The edges can be represented by an *adjacency matrix*, $\mathbf{A} \in \mathbb{R}^{|\mathcal{V}| \times |\mathcal{V}|}$, such that

$$A_{uv} = \begin{cases} 1 & \text{if } (u, v) \in \mathcal{E} \\ 0 & \text{otherwise} \end{cases}$$

2. Some interesting graph types:

- **Undirected:** $\forall u, v \in \mathcal{V}. (u, v) \in \mathcal{E} \iff (v, u) \in \mathcal{E}$ (i.e., $\mathbf{A}^\top = \mathbf{A}$)
- **Weighted:** provided *edge weight* w_{uv} for every edge $(u, v) \in \mathcal{E}$
- **Multirelational:** various *edge types*, i.e. $(u, t, v) \in \mathcal{E}$ if there exists an edge (u, v) linked by type t
- **Heterogeneous:** various *node types*

3. Machine learning tasks on graphs by domain:

- **Transductive:** training algorithm sees all observations, including the holdout observations
 - Task is to *propagate* labels from the training observations to the holdout observations
 - Also called *semi-supervised learning*
- **Inductive:** training algorithm only sees the training observations during training, and only sees the holdout observations for prediction

4. Node statistics:

- **Degree:** amount of edges the node is incident to:

$$d_u = \sum_{v \in \mathcal{V}} A_{uv}$$

- **Centrality:** a measure of how “central” the node is in the graph: how often do infinite random walks visit the node?

$$d_u = \lambda^{-1} \sum_{v \in \mathcal{V}} A_{uv} e_v$$

where $\mathbf{e} \in \mathbb{R}^{|\mathcal{V}|}$ is the largest eigenvector of \mathbf{A} , with corresponding eigenvalue λ

- **Clustering coefficient:** a measure of “clusteredness”: are neighbours connected amongst each other?

$$c_u = \frac{|\{(v_1, v_2) \in \mathcal{E} \mid v_1, v_2 \in \mathcal{N}(u)\}|}{\binom{d_u}{2}}$$

5. Graph Laplacian:

Let \mathbf{D} be the diagonal (out)-degree matrix of the graph, i.e., $D_{uu} = \sum_{v \in \mathcal{V}} A_{ij}$. Then:

- The *unnormalised* graph Laplacian: $\mathbf{L} = \mathbf{D} - \mathbf{A}$
- The *symmetric* graph Laplacian: $\mathbf{L}_{\text{sym}} = \mathbf{D}^{-\frac{1}{2}} \mathbf{L} \mathbf{D}^{-\frac{1}{2}} = \mathbf{I} - \mathbf{D}^{-\frac{1}{2}} \mathbf{A} \mathbf{D}^{-\frac{1}{2}}$
- The *random walk* graph Laplacian: $\mathbf{L}_{\text{RW}} = \mathbf{D}^{-1} \mathbf{L} = \mathbf{I} - \mathbf{D}^{-1} \mathbf{A}$

Properties:

- For undirected graphs, \mathbf{L} is *symmetric* ($\mathbf{L}^\top = \mathbf{L}$) and *positive semi-definite* ($\forall \mathbf{x} \in \mathbb{R}^{|\mathcal{V}|}. \mathbf{x}^\top \mathbf{L} \mathbf{x} \geq 0$)
- For undirected graphs:

$$\forall \mathbf{x} \in \mathbb{R}^{|\mathcal{V}|}. \mathbf{x}^\top \mathbf{L} \mathbf{x} = \frac{1}{2} \sum_{u \in \mathcal{V}} \sum_{v \in \mathcal{V}} A_{uv} (x_u - x_v)^2 = \sum_{(u,v) \in \mathcal{E}} (x_u - x_v)^2$$

- \mathbf{L} has $|\mathcal{V}|$ nonnegative eigenvalues: $\lambda_1 \geq \dots \geq \lambda_{|\mathcal{V}|} = 0$

6. Spectral clustering:

- Two-way cut: partition the graph into $\mathcal{A} \subseteq \mathcal{V}$ and its complement $\mathcal{A}_c \subseteq \mathcal{V}$:

$$\text{Cut}(\mathcal{A}) = |\{(u, v) \in \mathcal{E} \mid u \in \mathcal{A} \wedge v \in \mathcal{A}_c\}|$$

Ratio cut metric:

$$\text{RCut}(\mathcal{A}) = \text{Cut}(\mathcal{A}) \left(\frac{1}{|\mathcal{A}|} + \frac{1}{|\mathcal{A}_c|} \right)$$

- Minimising $\text{RCut}(\mathcal{A})$:

Let $\mathbf{a} \in \mathbb{R}^{|\mathcal{V}|}$ be a vector representing the cut \mathcal{A} , defined as follows:

$$a_u = \begin{cases} \sqrt{\frac{|\mathcal{A}_c|}{|\mathcal{A}|}} & \text{if } u \in \mathcal{A} \\ -\sqrt{\frac{|\mathcal{A}|}{|\mathcal{A}_c|}} & \text{if } u \in \mathcal{A}_c \end{cases}$$

Then

$$\mathbf{a}^\top \mathbf{L} \mathbf{a} = \sum_{(u,v) \in \mathcal{E}} (a_u - a_v)^2 = |\mathcal{V}| \text{RCut}(\mathcal{A})$$

Minimising $\mathbf{a}^\top \mathbf{L} \mathbf{a}$ corresponds to minimising $\text{RCut}(\mathcal{A})$ (NP-hard as the constraint is discrete)

- Relaxing: minimise $\mathbf{a}^\top \mathbf{L} \mathbf{a}$ subject to $\mathbf{a} \perp \mathbf{1}$ and $\|\mathbf{a}\|^2 = |\mathcal{V}|$
Rayleigh–Ritz Theorem: The solution is exactly the second-smallest eigenvector of \mathbf{L}
To obtain the cut, place u into \mathcal{A} or \mathcal{A}_c depending on the sign of a_u
- Can be generalised to k -clustering

2 Permutation Invariance and Equivariance

1. Informal definitions:

- **Permutation invariance:** applying a permutation matrix does not modify the result
- **Permutation equivariance:** transformation preserves the node order
- **Locality:** signal remains stable under slight deformations of the domain

2. Setup:

- **Node feature matrix:** $\mathbf{X} = [\mathbf{x}_1 \ \cdots \ \mathbf{x}_{|\mathcal{V}|}]^\top \in \mathbb{R}^{|\mathcal{V}| \times k}$, where $\mathbf{x}_i \in \mathbb{R}^k$ is the features of node i
- **(1-hop) neighbourhood** of node i : $\mathcal{N}_i = \{j \mid (i, j) \in \mathcal{E} \vee (j, i) \in \mathcal{E}\}$
- **Neighbourhood features:** $\mathbf{X}_{\mathcal{N}_i} = \{\{\mathbf{x}_j \mid j \in \mathcal{N}_i\}\}$
- **Permutation matrix:** a $|\mathcal{V}| \times |\mathcal{V}|$ binary matrix that has exactly one entry of 1 in every row and column, and 0s elsewhere: $\mathbf{P} = [\mathbf{e}_{\pi(1)} \ \cdots \ \mathbf{e}_{\pi(|\mathcal{V}|)}]^\top$

3. Learning on sets:

- $f(\mathbf{X})$ is *permutation invariant* if for all permutation matrices \mathbf{P} : $f(\mathbf{P}\mathbf{X}) = f(\mathbf{X})$
- $\mathbf{F}(\mathbf{X})$ is *permutataion equivariant* if for all permutation matrices \mathbf{P} : $\mathbf{F}(\mathbf{P}\mathbf{X}) = \mathbf{P}\mathbf{F}(\mathbf{X})$
- Locality on sets: transform every node in isolation, through a shared function ψ : $\mathbf{h}_i = \psi(\mathbf{x}_i)$
Stacking \mathbf{h}_i into a matrix yields $\mathbf{H} = \mathbf{F}(\mathbf{X})$:

$$\mathbf{F}(\mathbf{X}) = \begin{bmatrix} - & \psi(\mathbf{x}_1) & - \\ & \vdots & \\ - & \psi(\mathbf{x}_{|\mathcal{V}|}) & - \end{bmatrix}$$

- Deep Sets (Zaheer *et al.*, NIPS 2017):

$$f(\mathbf{X}) = \phi \left(\bigoplus_{i \in \mathcal{V}} \psi(\mathbf{x}_i) \right)$$

Universality of Deep Sets: any permutation invariant model can be expressed as a Deep Sets

4. Learning on graphs:

- $f(\mathbf{X})$ is *permutation invariant* if for all permutation matrices \mathbf{P} : $f(\mathbf{P}\mathbf{X}, \mathbf{P}\mathbf{A}\mathbf{P}^\top) = f(\mathbf{X}, \mathbf{A})$
- $\mathbf{F}(\mathbf{X})$ is *permutataion equivariant* if for all permutation matrices \mathbf{P} : $\mathbf{F}(\mathbf{P}\mathbf{X}, \mathbf{P}\mathbf{A}\mathbf{P}^\top) = \mathbf{P}\mathbf{F}(\mathbf{X}, \mathbf{A})$
- Locality on graphs: apply a local function ϕ over all neighbourhoods:

$$\mathbf{F}(\mathbf{X}, \mathbf{A}) = \begin{bmatrix} - & \phi(\mathbf{x}_1, \mathbf{X}_{\mathcal{N}_1}) & - \\ & \vdots & \\ - & \phi(\mathbf{x}_{|\mathcal{V}|}, \mathbf{X}_{\mathcal{N}_{|\mathcal{V}|}}) & - \end{bmatrix}$$

To ensure permutation equivariance, it is sufficient that ϕ is permutation invariant in $\mathbf{X}_{\mathcal{N}_i}$

Appendix: Mathematical Notations

a	A scalar (integer or real)
\mathbf{a}	A vector
\mathbf{A}	A matrix
\mathcal{A} or $\{\cdot\}$	A set
$\{\{\cdot\}\}$	A multiset
$ \mathcal{A} $	Cardinality of set \mathcal{A}
\mathbb{R}	The set of real numbers
a_i	Element i of vector \mathbf{a} , with indexing starting at 1
A_{ij}	Element i, j of matrix \mathbf{A} , with indexing starting at 1
f	A function
\mathbf{F}	A matrix-valued function
π	A permutation
ϕ, ψ, \dots	Learnable functions (e.g., MLPs)
\oplus	A permutation-invariant operator (e.g., sum, mean, min, max)