Graph contrastive clustering

Problem formulation:

Unlabeled data: $I = \{I_1, \cdots I_N\}$

Embedding $\phi_\theta : I_i \rightarrow (\underbrace{z_i}_{\text{Rep feats.}}, p)$ ↳ cluster group.

No of cluster.

$$\sum_{j=1}^{k} p_{ij} = 1$$

Cluster Assignment:

$$l_i = \arg\max_j (p_{ij}), \quad \boxed{1 \leq j \leq k}$$

Graph Contrastive:

$$\mathcal{G} = (V, E)$$

$$V = \{v_1, v_2 \cdots v_N\}$$

Adjacency Matrix A with $A_{ij} = \begin{cases} 1 & : (v_i, v_j) \in E \\ 0 & \text{else} \end{cases}$

Adjacency Ma[illegible] [illegible] else

Degree Matrix: $D = \begin{bmatrix} d_1 & 0 & \cdots & 0 \\ 0 & d_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & d_N \end{bmatrix}$

Laplacian : $L = I - D^{-1/2} A D^{-1/2}$

$$L_{ij} = -\frac{A_{ij}}{\sqrt{d_i d_j}} \; ; \; i \neq j$$

Representation features:

x_i & x_j close if $A_{ij} > 0$

x_i & x_j far away if $A_{ij} = 0$

Similarity:

$$S_{intra} = \sum_{L_{ij} < 0} -L_{ij} \, S(x_i, x_j)$$

$$S_{inter} = \sum S(x_i, x_j)$$

$L_{ij}' = 0$

Now, GC loss :

$$\mathcal{L}_{gc} = -\frac{1}{N}\sum_{i=1}^{N} \log\left(\frac{\sum_{L_{ij}'<0} -L_{ij}\, S(x_i, x_j)}{\sum_{L_{ij}'=0} S(x_i, x_j')}\right)$$

<u>Graph Construction</u>:

Embedding

$$(z_1^t, z_2^t, \ldots z_N^t) = (\phi_\theta^t(I_1) \ldots\ldots)$$

$$\bar{z}_i^t = \frac{(1-\alpha)\bar{z}_i^{t-1} + \alpha z_i^t}{\|(1-\alpha) z_i^{t-1} + \alpha z_i^t\|_2}; \quad i = 1 \ldots N$$

<u>Construction of graph</u>:

neighborhood of $\bar{z}$

$$A_{ij}^t = \begin{cases} 1 \rightarrow; & \boxed{\text{if } \bar{z}_j^t \in \mathcal{N}^k(\bar{z}_i, t) \text{ or } \bar{z}_i^t \in \mathcal{N}(\bar{z}_j, t)} \\ 0 & \rightarrow \text{otherwise} \end{cases}$$

$$S(x_i, x_j) = e^{-\|x_i - x_j\|_2^2 / c}$$

$$= e^{x_i' x_j' / \tau}$$

Representation Graph Cluster loss:

$$\mathcal{L}_{RGC}^{(t)} = -\frac{1}{N} \sum_{i=1}^{N} \log\left(\frac{\sum_{L_{ij}' < 0} -L_{ij}^{t} \, e^{(z_i', z_j' / \tau)}}{\sum_{L_{ij} \neq 0} e^{z_i' z_j' / \tau}} \right)$$

Assignment GC:

$I' = \{I_1', \dots, I_N'\}$ Augmented version.

$$\tilde{I}' = \left\{ \tilde{I}_1', \dots \tilde{I}_n' \right\} \leftarrow \left[\begin{array}{l} \text{trax of Random} \\ \text{neighbour hood } I_i' \text{ image} \\ \text{from } A^t \end{array} \right.$$

$$P' = \begin{bmatrix} P_1' \\ \vdots \\ P_N' \end{bmatrix}_{N \times k} \qquad \tilde{P}' = \begin{bmatrix} P'_{RN(I_1)} \\ \vdots \\ P'_{RN(I_N)} \end{bmatrix}_{N \times k}$$

$\Big\{ RN(I_i) \rightarrow$ Random neighborhood image of I_i

Reformulating p' & $\tilde{p}'$ to $\boxed{\text{column vector}}$

$$q' = [q'_1 \;\cdots\; q'_k]_{N \times k}$$

which picture in I' is assigned to i'

$$\tilde{q}' = [\tilde{q}'_1, \;\cdots\; \tilde{q}'_k]_{N \times k}$$

$$\mathcal{L}_{AGC} = -\frac{1}{k} \sum_{i=1}^{k} \log \left(\frac{e^{q'_i \tilde{q}'_i / \tau}}{\sum_{j=1}^{k} e^{q'_i \tilde{q}'_j / \tau}} \right)$$

cluster regularization loss:

$$\mathcal{L}_{CR} = \log(k) - H(z)$$

$$z_{i'} = \frac{\sum_{j=1}^{N} q_{ij}'}{\sum_{j} \sum_{k} q_{jk}}$$

$$q = [q_1 \;\cdots\; q_k]$$

k min Prob

// Assign

$$\boxed{\mathcal{L} = \mathcal{L}_{PGC} + \lambda \mathcal{L}_{AGC} + \eta \mathcal{L}_{CR}}$$