

ICLR 2019

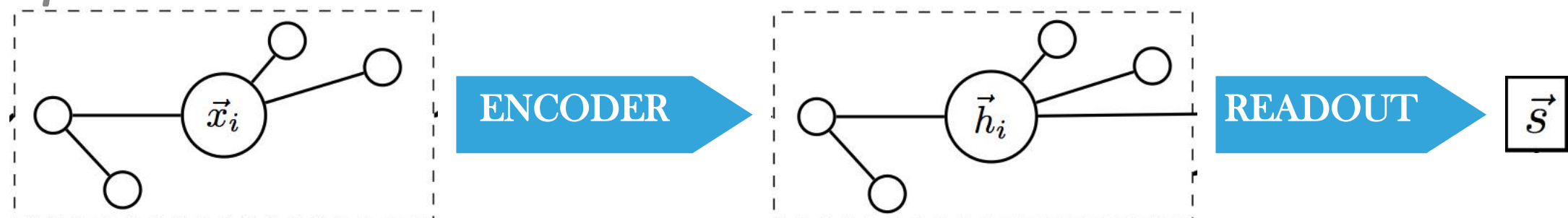
DEEP GRAPH INFOMAX

MOTIVATION

- ▶ *Most successful methods use supervised learning while most graph data is unlabeled.*
- ▶ *Random walk-based methods over-emphasize proximity information at the expense of structural information.*
- ▶ *High dependence on hyperparameter choice*

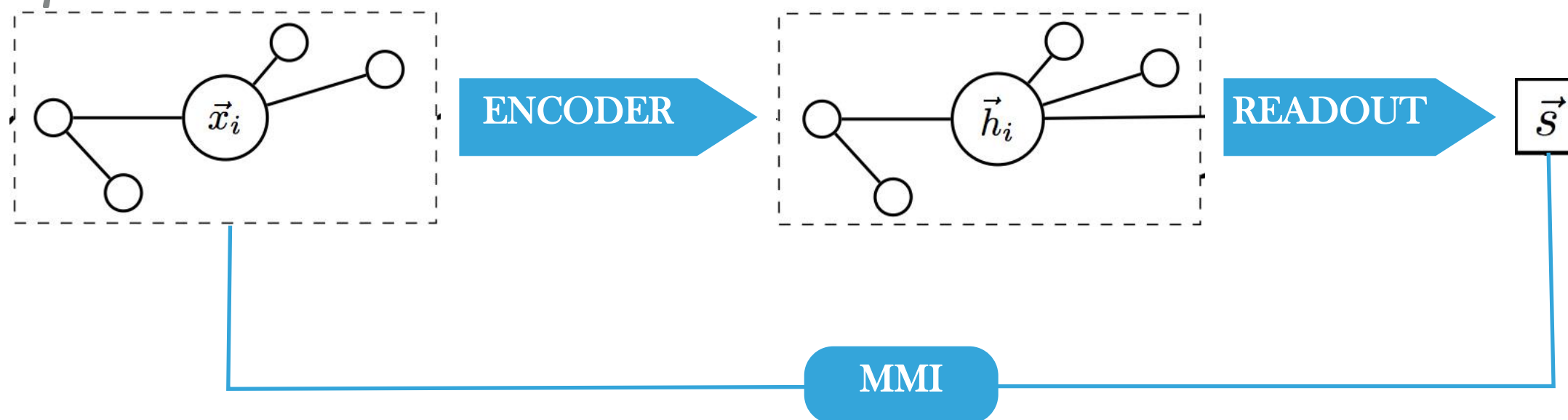
KEY POINT

- ▶ A general approach for learning node *embeddings* in an *unsupervised* manner.
- ▶ Maximize mutual information between a high-level “global” representation and “local” parts of the input.



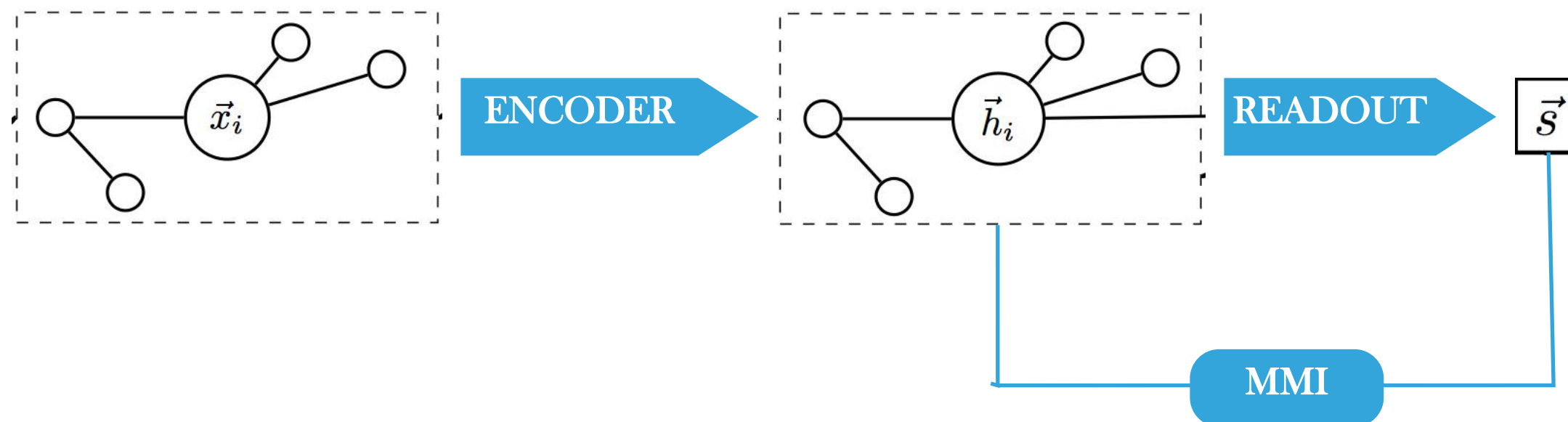
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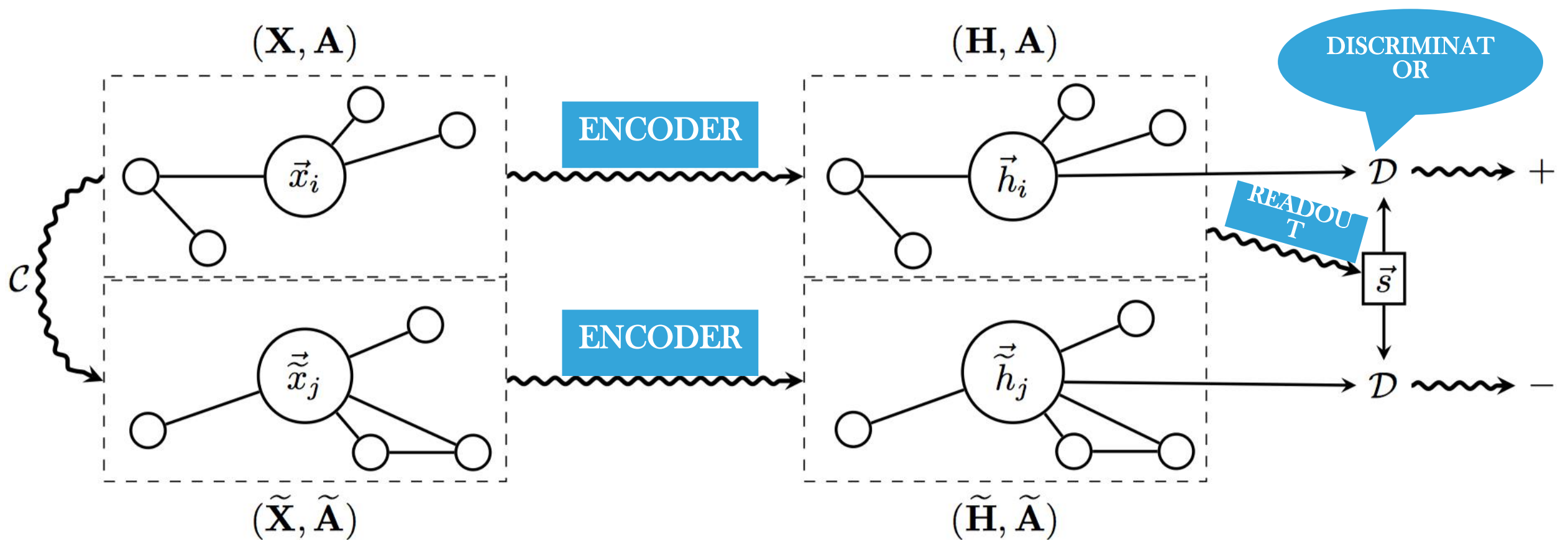


MUTUAL INFORMATION (MI)

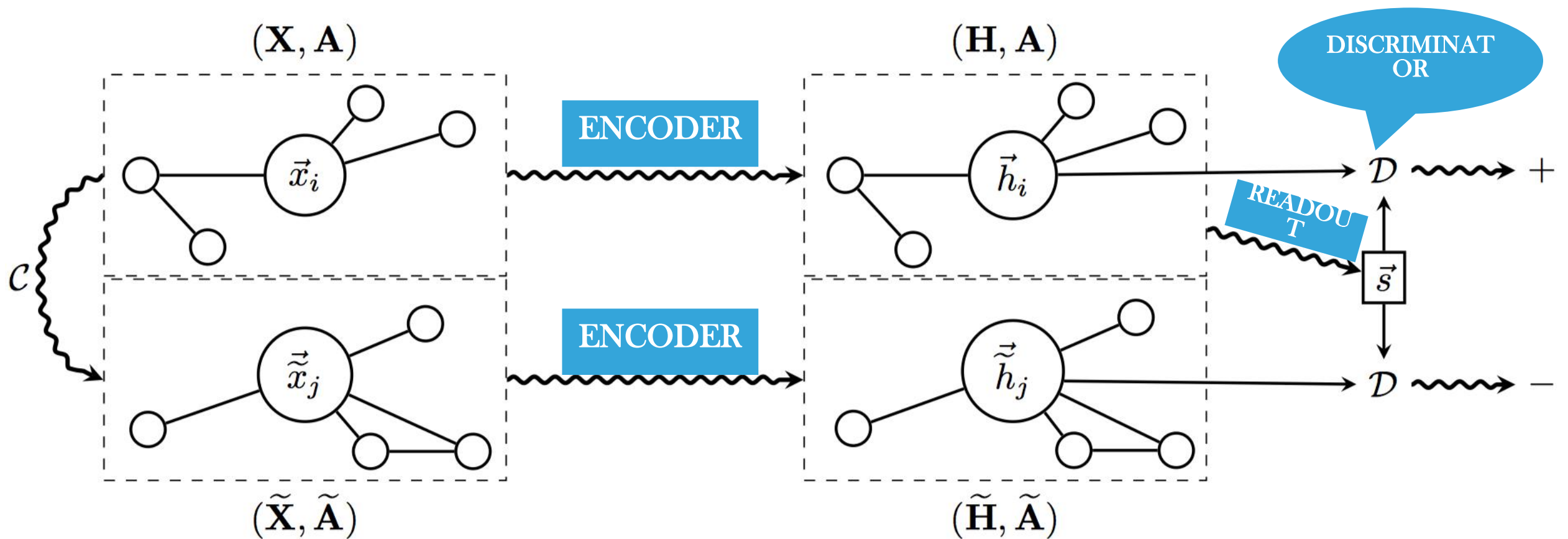
- ▶ 互信息表示两个变量 X 与 Y 是否有关系，以及关系的强弱
- ▶ 通过考察其联合概率分布 $p(X, Y)$ 与边缘概率分布乘积 $p(X)p(Y)$ 之间的 KL 散度来判断独立程度 $I(X, Y) = KL(p(X, Y) // p(X)p(Y))$



OVERVIEW OF DEEP GRAPH INFOMAX



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$$\mathcal{L} = \frac{1}{N + M} \left(\sum_{i=1}^N \mathbb{E}_{(\mathbf{X}, \mathbf{A})} \left[\log \mathcal{D} \left(\vec{h}_i, \vec{s} \right) \right] + \sum_{j=1}^M \mathbb{E}_{(\tilde{\mathbf{X}}, \tilde{\mathbf{A}})} \left[\log \left(1 - \mathcal{D} \left(\vec{\tilde{h}}_j, \vec{s} \right) \right) \right] \right)$$

EXPERIMENT

- ▶ *Encoder*
 - ▶ Transductive learning (GCN)
 - ▶ Inductive learning on large graphs (GraphSAGE-GCN)
- ▶ *Readout* $\mathcal{R}(\mathbf{H}) = \sigma \left(\frac{1}{N} \sum_{i=1}^N \vec{h}_i \right)$
- ▶ *Discriminator* $\mathcal{D}(\vec{h}_i, \vec{s}) = \sigma \left(\vec{h}_i^T \mathbf{W} \vec{s} \right)$