GNNExplainer论文分享

1. Overview

- 一句话概括："We formulate GNNEXPLAINER as an optimization task that maximizes the mutual information between a GNN’s prediction and distribution of possible subgraph structures."

2. 背景

2.1 graph embedding问题定义

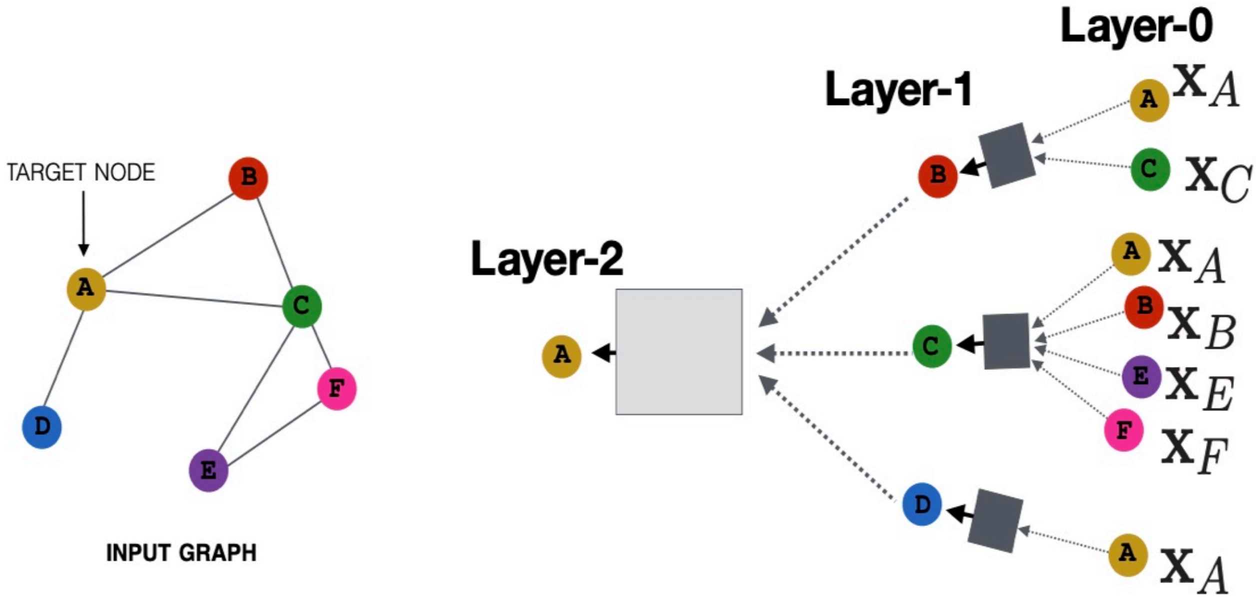
Definition 4. *(Graph embedding) Given a graph* $G = (V, E)$*, a graph embedding is a mapping* $f : v_i \rightarrow \boldsymbol{y_i} \in \mathbb{R}^d \ \forall i \in [n]$ *such that* $d \ll |V|$ *and the function* f *preserves some proximity measure defined on graph* G*.*

- 定义：求图上节点的映射，使得映射后的节点满足图结构上的”相似“
- 怎么定义相似？基于图的应用场景定义
- 以社交网络为例：
    - 节点间有边相连（first-order proximity），人以类聚物以群分
    - 节点的邻居重叠（second-order proximity），共同好友多
    - 节点的特征（node feature）相似，爱好相同
    - ……

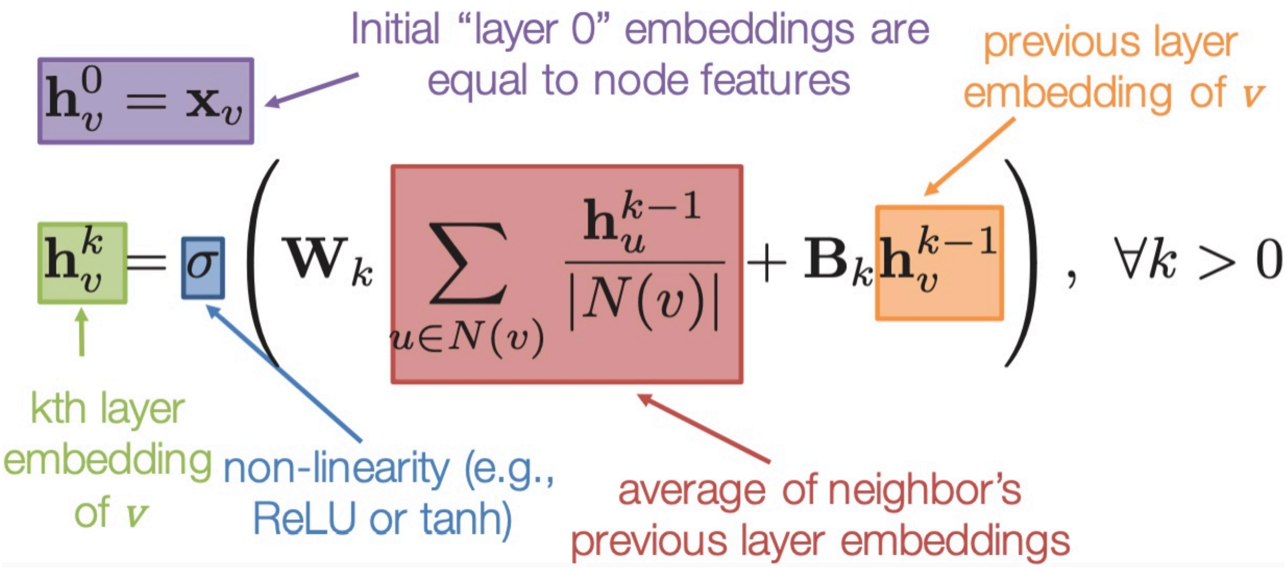
2.2 Graph Neural Network(GNN)

- 迭代地延边传播节点间的神经网络信号，巧妙融合了节点特征和图上信号传播的思想
- inductive learning：参数共享，训练好的网络参数可直接用于新增节点的预测

直观上



数学上



2.3 GNN计算流程

GCN:

$$H^{(l+1)} = \sigma(H^{(l)} W_0^{(l)} + D^{-\frac{1}{2}} A D^{-\frac{1}{2}} H^{(l)} W_1^{(l)})$$

GraphSage:

$$h_v^K = \sigma([W_k AGG(\{h_u^{k-1}, \forall u \in N(v)\}), B_k h_v^{k-1}])$$

1. MSG: 节点对(v_i, v_j)在第l层的传递信号可以用$m_{ij}^l = MSG(h_i^{l-1}, h_j^{l-1}, r_{ij})$其中$h_i^{l-1}$表示$l-1$层的节点编码（信号），$r_{ij}$表示节点间关联。

2. AGG: 节点v_i聚合邻居传递的信号，$M_i^l = AGG(\{m_{ij}^l, \forall v_j \in N(v_i)\})$。
3. $UPDATE$: 节点v_i结合AGG和自身在上一层的编码，非线性变化得l层编码 $h_i^l = UPDATE(M_i^l, h_i^{l-1})$。

本文意在建模解释上述流程描述的任何GNN预测。

2.4 理解GNN预测的意义

- 风控场景模型结果的可解释性极为重要，提高业务对技术的信任
- 提高模型的透明度，赋能业务理解黑产行为/社区生态行为
- 提高开发者对GNN网络结构的理解，降低调试成本，便于debug

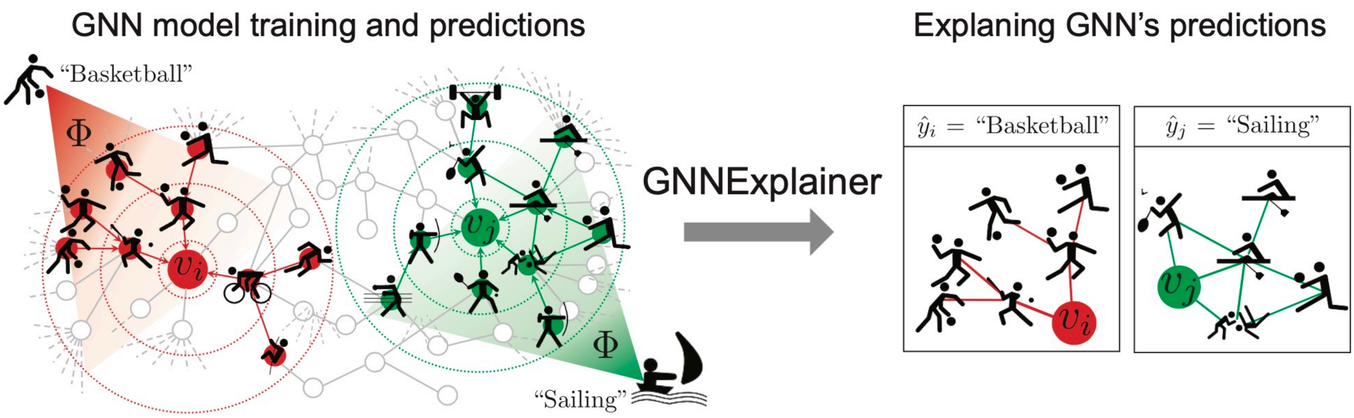


Figure 1: GNNEXPLAINER provides interpretable explanations for predictions made by any GNN model on any graph-based machine learning task. Shown is a hypothetical node classification task where a GNN model Φ is trained on a social interaction graph to predict future sport activities. Given a trained GNN Φ and a prediction $\hat{y}_i$ = "Basketball" for person v_i, GNNEXPLAINER generates an explanation by identifying a small subgraph of the input graph together with a small subset of node features (shown on the right) that are most influential for $\hat{y}_i$. Examining explanation for $\hat{y}_i$, we see that many friends in one part of v_i's social circle enjoy ball games, and so the GNN predicts that v_i will like basketball. Similarly, examining explanation for $\hat{y}_j$, we see that v_j's friends and friends of his friends enjoy water and beach sports, and so the GNN predicts $\hat{y}_j$ = "Sailing."

2.5 问题的数学表述

对给定节点v，GNN模型Φ的预测可表示为

$$\hat{y} = \Phi(G_c(v), X_c(v)).$$

其中G_c表示v的计算图，X_c表示图上的节点特征。即GNN模型Φ可表示为条件分布 $P_\Phi(Y|G_c, X_c)$。

那么解释预测$\hat{y}$的问题可以通过求解下式表述：

$$\arg \max_{G_S \subset G_c(v), X_S^F \subset X_c(v)} MI(Y, (G_S, X_S^F))$$

其中MI表示互信息，X_S表示子图G_S的节点特征集合，F为节点特征集合上的掩码。我们希望找到最主要影响预测结果$\hat{y}$的子图和对应节点特征的子集，输出作为解释预测的论据。这种影响通过互信息（mutual information）量化描述，即找到对随机变量Y分布影响最大的因子。

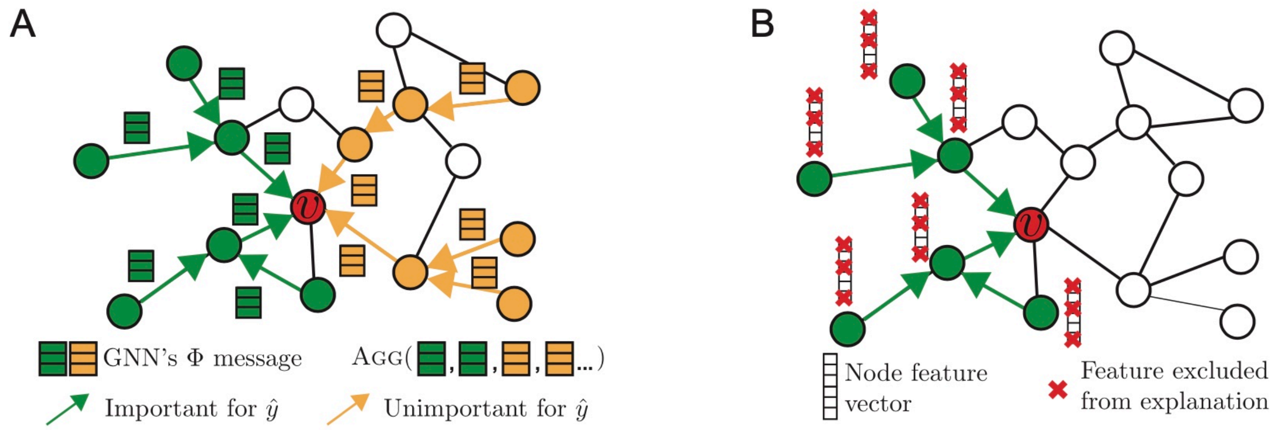


Figure 2: **A.** GNN computation graph G_c (green and orange) for making prediction $\hat{y}$ at node v. Some edges in G_c form important neural message-passing pathways (green), which allow useful node information to be propagated across G_c and aggregated at v for prediction, while other edges do not (orange). However, GNN needs to aggregate important as well as unimportant messages to form a prediction at node v, which can dilute the signal accumulated from v's neighborhood. The goal of GNNEXPLAINER is to identify a small set of important features and pathways (green) that are crucial for prediction. **B.** In addition to G_S (green), GNNEXPLAINER identifies what feature dimensions of G_S's nodes are important for prediction by learning a node feature mask.

注意到$MI(Y,(G_S,X_S^F))=H(Y)-H(Y|G=G_S,X=X_S^F)$，对给定的GNN模型$H(Y)$固定，那么原问题转化为最小化条件熵

$$H(Y|G=G_S,X=X_S^F)=-\mathbf{E}_{Y|G_S,X_S^F}[\log P(Y|G=G_S,X=X_S^F)].$$

2.6 求解

2.6.1 不筛选节点特征

即$X_S^F=X_S=X_S(G_S)$时，记G_S服从随机图分布$\mathcal{G}$，那么优化目标可表示为

$$\min_{\mathcal{G}} \mathbf{E}_{G_S\sim\mathcal{G}}[H(Y|G=G_S,X=X_S)]$$

在凸性假设下由Jensen's Inequality有上界：

$$\min_{\mathcal{G}} H(Y|G=\mathbf{E}_{G_S\sim\mathcal{G}}[G_S],X=X_S).$$

不过NN模型不满足凸性，这里作者表示实验表明加上*正则项*（参考2.6.3）后，由目标函数得到的局部极小值也很好用。

这里直接用exact inference求分布$\mathcal{G}$使目标函数最小的计算复杂度高，因G_c有指数量级的子图G_S。假设隐变量e_{ij}相互独立，采用mean-field variational family近似分布$\mathcal{G}$有

$$P_{\mathcal{G}}(G_S) = \prod_{(j,k)\in G_c} A_S[j,k] \;\; s.t. \;\; A_S \in [0,1]^{n\times n}, \;\; \forall j,k \; A_S[j,k] \leq A_c[j,k].$$

这里A_S是fractional adjacency matrix，$P(e_{jk} \in G_S) = A_S[j,k]$。因此在近似分布$P_{\mathcal{G}}$下，有$\mathbf{E}_{G_S\sim\mathcal{G}}[G_S] \approx A_c \odot \sigma(M)$，$M \in \mathbf{R}^{n\times n}$就是我们需要学习的参数矩阵（mask）。通过sigmoid函数映射到$[0,1]$上的概率。

在一些应用中，我们往往只关心为什么给节点打上一类标记（如只关心”坏人“的预测）。此时可以把优化目标改为交叉熵，用梯度下降优化：

$$\min_M -\sum_{c=1}^{C} \mathbb{I}[y=c] \log P_\Phi(Y=y|G=A_c \odot \sigma(M), X=X_c).$$

最后输出解释子图G_S可通过对M设定阈值后移除低于阈值的边实现。

2.6.2 筛选节点特征

$F \in \{0,1\}^d$表示节点特征集合上的掩码，即

$$X_S^F = \{x_j^F | v_j \in G_S\}, \quad x_j^F = [x_{j,t_1}, \ldots, x_{j,t_k}] \; for \; F_{t_i} = 1.$$

此时最大化互信息目标函数表示为：

$$MI(Y,(G_S,F)) = H(Y) - H(Y|G=G_S, X=X_S^F).$$

同上节，记$X_S^F = X_S \odot F$，用reparametrization tricks有$X = Z + (X_S - Z) \odot F$，$Z$为基于经验分布的采样，使梯度可以传到参数矩阵$F$。

2.6.3 正则项

实际应用中为了使梯度下降收敛到较好的局部最优解，可对参数矩阵$\sigma(M)$和F取element-wise entropy加入loss使参数$\sigma(M)$和F稀疏化，即$L_{entropy} = \frac{1}{n^2}\sum_{j,k} H(\sigma(M)_{j,k})$。

```
# entropy
mask_ent = -mask * torch.log(mask) - (1 - mask) * torch.log(1 - mask)
mask_ent_loss = self.coeffs["ent"] * torch.mean(mask_ent)
```

```python
feat_mask_ent = - feat_mask             \
                * torch.log(feat_mask)  \
                - (1 - feat_mask)       \
                * torch.log(1 - feat_mask)

feat_mask_ent_loss = self.coeffs["feat_ent"] * torch.mean(feat_mask_ent)
```

2.6.4 multi-instance explanations through graph prototypes

3. 拓展

3.1 weighted graph

Algorithm 1 Optimize mask for weighted graph

Input: 1. $G_c(u)$, computation graph of node u; 2. Pre-trained GNN model Φ; 3. y_u, node u's real label; 4. $\mathcal{M}$, learn-able mask; 5. K, number of optimization iterations; 6. L, number of layers of GNN.

$\mathcal{M} \leftarrow$ randomize parameters ▷ initialize, $\mathcal{M} \in [0,1]^Q$
$\mathbf{h}_v^{(0)} \leftarrow \mathbf{x}_v$, for $v \in G_c(u)$
for $k = 1$ to K **do**
  $\mathcal{M}_{vw} \leftarrow \frac{exp(\mathcal{M}_{vw} e_{vw})}{\sum_v exp(\mathcal{M}_{vw} e_{vw})}$ ▷ renormalize mask
  for $l = 1$ to L **do**
    $\mathbf{m}_{vu}^{(l)} \leftarrow W_1^{(l-1)} \mathbf{h}_v^{(l-1)}$ ▷ message
    $M_u^{(l)} \leftarrow \sum_v g(\mathcal{M}_{vu} \mathbf{m}_{vu}^{(l)}, \mathbf{h}_u^{(l-1)})$ ▷ aggregate
    $\mathbf{h}_u^{(l)} \leftarrow \sigma(W_0 \mathbf{h}_u^{(l-1)} + M_u^{(l)})$ ▷ update
  end for
  $\hat{\mathbf{y}}_u \leftarrow softmax(\mathbf{h}_u^{(L)})$ ▷ predict on masked graph
  $loss \leftarrow crossentropy(\mathbf{y}_u, \hat{\mathbf{y}}_u) + regularizations$
  $\mathcal{M} \leftarrow optimizer(loss, \mathcal{M})$ ▷ update mask
end for
Return: $\mathcal{M}$

4. 实验

见论文

5. 代码分析

https://github.com/RexYing/gnn-model-explainer
待填坑

6. 总结

7. 参考文献

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