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Learning Graph Representations with Embedding Propagation

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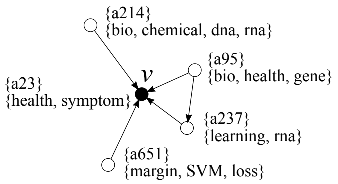
MOTIVATION



A graph $G = (V, E)$ with k label types

Motivation: Graph-structured data occurs in numerous application domains such as social networks, bioinformatics and relational knowledge bases. Nodes may have an arbitrary number of label types, and these label types may be heterogeneous (node entities, text, images...).

Contributions: We propose **embedding propagation** (EP), an unsupervised learning framework that supports arbitrary label types.

Results: With significantly fewer parameters and hyperparameters an instance of EP is competitive with and often outperforms state-of-the-art unsupervised and semi-supervised learning algorithms on a range of benchmark node classification data sets.

EMBEDDING PROPAGATION (EP): THE FRAMEWORK

Our novel **embedding propagation** framework learns label and node representations by passing messages between neighbors.

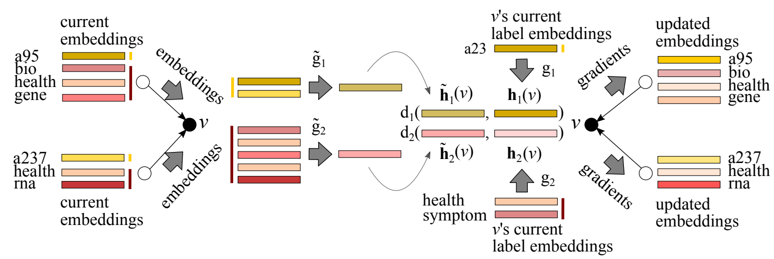
Label Representations

- Let $\boldsymbol{\ell} \in \Re^d$ be the representation of label ℓ, and $\mathtt{f}$ be a differentiable embedding function
- For labels of label type i, we apply a learnable embedding function $\boldsymbol{\ell} = \mathtt{f}_i(\ell)$
- $\mathbf{h}_i(v)$ is the *embedding of label type i* for vertex v:
$$\mathbf{h}_i(v) = \mathtt{g}_i\left(\{\boldsymbol{\ell} \mid \ell \in \text{labels of type } i \text{ associated with vertex } v\}\right)$$
- $\widetilde{\mathbf{h}}_i(v)$ is the *reconstruction of the embedding of label type i* for vertex v:
$$\widetilde{\mathbf{h}}_i(v) = \widetilde{\mathtt{g}}_i\left(\{\boldsymbol{\ell} \mid \ell \in \text{labels of type } i \text{ associated with the neighbors of vertex } v\}\right)$$

Node Representations

- Let $\mathbf{v}$ be the representation of a vertex v computed by applying a function $\mathtt{r}$ on the representations of v's labels:
$$\mathbf{v} = \mathtt{r}\left(\{\boldsymbol{\ell} \mid \ell \in \text{all labels associated with vertex } v\}\right)$$

EP message passing



Learning objective for each label type $i \in \{1, \ldots, k\}$:

$$\min \mathcal{L}_i = \min \sum_{v \in V} \sum_{u \in V \setminus \{v\}} \left[\gamma + \mathtt{d}_i\left(\widetilde{\mathbf{h}}_i(v), \mathbf{h}_i(v)\right) - \mathtt{d}_i\left(\widetilde{\mathbf{h}}_i(v), \mathbf{h}_i(u)\right)\right]_+$$

where $\mathtt{d}_i$ is the Euclidean distance, $[x]_+$ is the positive part of x, and $\gamma > 0$ is a margin hyperparameter.

A simple instance of EP

EP-B

- $\mathtt{f}_i$ are embedding lookup tables
- $\mathtt{g}_i(\mathbf{H}) = \widetilde{\mathtt{g}}_i(\mathbf{H}) = \frac{1}{|\mathbf{H}|}\sum_{\mathbf{h} \in \mathbf{H}} \mathbf{h}$ for all label types i
- $\mathbf{v} = \mathtt{concat}\left[\mathbf{h}_1(v), ..., \mathbf{h}_k(v)\right]$
- **Inductive** setting: $\mathbf{v} = \mathtt{concat}\left[\widetilde{\mathbf{h}}_1(v), ..., \widetilde{\mathbf{h}}_k(v)\right]$

For a graph without node attributes.

Method	#params	#hyperparams
DeepWalk [Perozzi et al.,2014]	$2d\|V\|$	4
node2vec [Grover et al.,2016]	$2d\|V\|$	6
LINE [Tang et al.,2015]	$2d\|V\|$	2
Planetoid [Yang et al., 2016]	$\gg 2d\|V\|$	≥ 6
Ep-B	$d\|V\|$	2

EVALUATION

Node classification:

- The input is a graph (with or without attributes)
- A fraction of the nodes is assigned a class label
- The output is an assignment of class labels to the test nodes
- EP is classifier agnostic
- In fairness to existing unsupervised works, we opt for logistic regression trained with node representations $\mathbf{v}$

Transductive setting

Method	Cora	Citeseer	Pubmed
EP-B	78.0% ± 1.5%	**71.0% ± 1.3%**	**79.6% ± 2.1%**
DW+BoW	76.1% ± 2.1%	61.9% ± 2.3%	77.8% ± 2.2%
Planetoid-T	71.9% ± 5.3%	58.6% ± 6.3%	74.5% ± 4.9%
GCN	**79.6% ± 2.0%**	69.2% ± 1.2%	77.3% ± 2.7%
DeepWalk	71.1% ± 2.7%	47.6% ± 2.3%	73.5% ± 3.0%
BoW Feat	58.6% ± 0.7%	58.1% ± 1.7%	70.5% ± 2.9%

Inductive setting

Method	Cora	Citeseer	Pubmed
EP-B	**73.1% ± 1.7%**	**68.6% ± 1.7%**	**79.9% ± 2.3%**
DW-I+BoW	68.3% ± 1.7%	59.5% ± 2.5%	74.9% ± 1.2%
Planetoid-I	64.8% ± 3.7%	62.0% ± 3.8%	75.7% ± 4.2%
GCN-I	67.7% ± 2.1%	63.4% ± 1,0%	73.5% ± 2.5%
BoW Feat	58.6% ± 0.7%	58.1% ± 1.7%	70.5% ± 2.9%