Lovász Convolutional Networks

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Problem Setting

Semi-Supervised Learning on Graph: Given a graph $G(V, E)$, we are given the labels ($\{0, 1\}$ in the case of binary classification) of a subset of nodes ($m < n$) of V and the goal is to predict the labels of the remaining nodes as accurately as possible.

Contributions

- Our proposed method LCN combines the power of using the Lovász embeddings with GCNs.
- We analyze various types of graphs and identify the classes of graphs where LCN performs much better than existing methods.
- We demonstrate that by keeping the optimal coloring (a global property) fixed, and increasing the number edges in the graph (local structure), LCNs outperforms traditional GCNs.
- We show significant improvement using LCNs than state of the art algorithms.

Motivation

Coloring Fraction

- Graph: $\mathbf{G} = (V, E)$
- $\chi(\tilde{\mathbf{G}})$: Optimal coloring of the complement graph.
- $\boldsymbol{n_d}$: Number of edges in G such that the pair of nodes each edge connects have different colors w.r.t $\chi(\tilde{G})$.
- $\boldsymbol{n_t}$: Total number of pairs of nodes in G such that the nodes in each pair have different colors w.r.t $\chi(\tilde{G})$.
- Coloring fraction: $\beta(G) = \frac{n_d}{n_t}$.

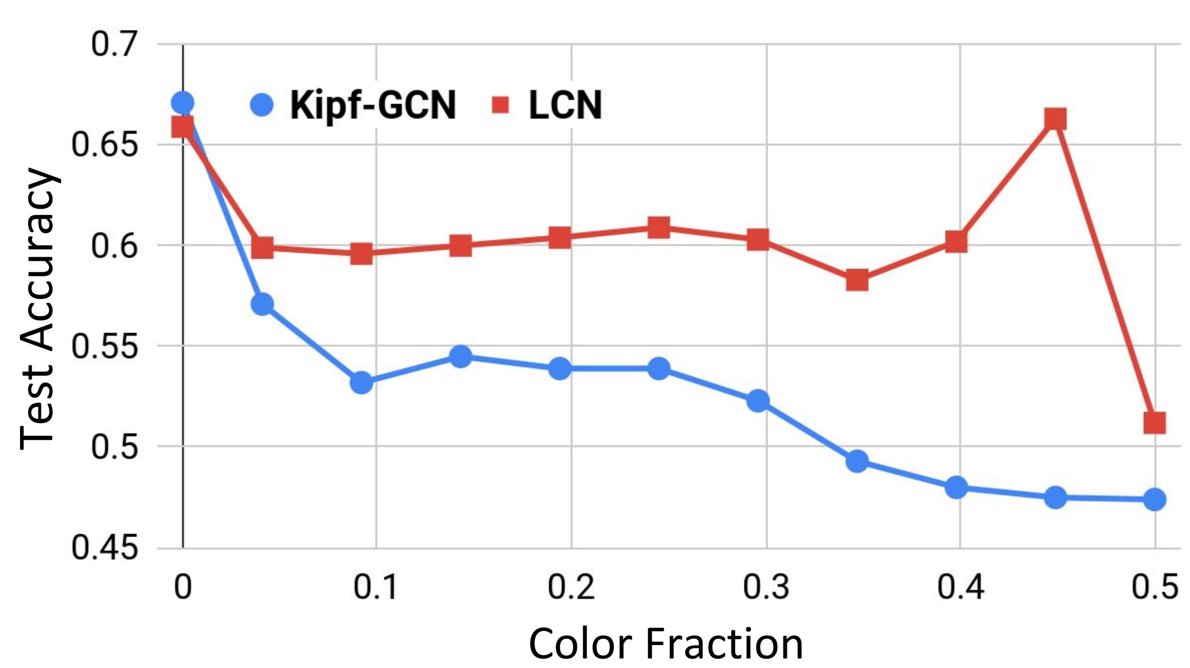

Figure 1: Variation of test accuracy for GCN and LCN - with variation in the graph structure.

Proposition

- Graph: $G(V, E)$
- $\beta(G)$: Coloring fraction of G.
- $|\chi(\bar{G})|$: Chromatic number of the complement of G.
- G' : The graph obtained from G by removing a set of edges whose nodes have different colors w.r.t the optimal coloring of $\bar{G}$. Then,

$$\chi(\bar{G}') = \chi(\bar{G}) \quad \text{whereas} \quad \beta(G') < \beta(G)$$

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Lovasz Orthonormal Embeddings

Definition: An orthogonal embedding of a graph $G(V, E)$ with $|V| = n$, is a matrix $\mathbf{U} = [\vec{u}_1, \ldots, \vec{u}_n] \in \mathbb{R}^{d \times n}$ such that $\vec{u}_i^\top \vec{u}_j = 0$ whenever $(i, j) \notin E$ and $\vec{u}_i \in \mathcal{S}^{d-1}\ \forall i \in [n]$.

- **Lovasz Kernel**: $K_{Lov} = \mathbf{U}\mathbf{U}^\mathbf{T}$, where $\mathbf{U}$ is the orthonormal Embeddings of G.
- **KLS Kernel**: $\mathbf{K}_{LS} = \frac{\mathbf{A}}{-\lambda_{\min}(\mathbf{A})} + \mathbf{I}$

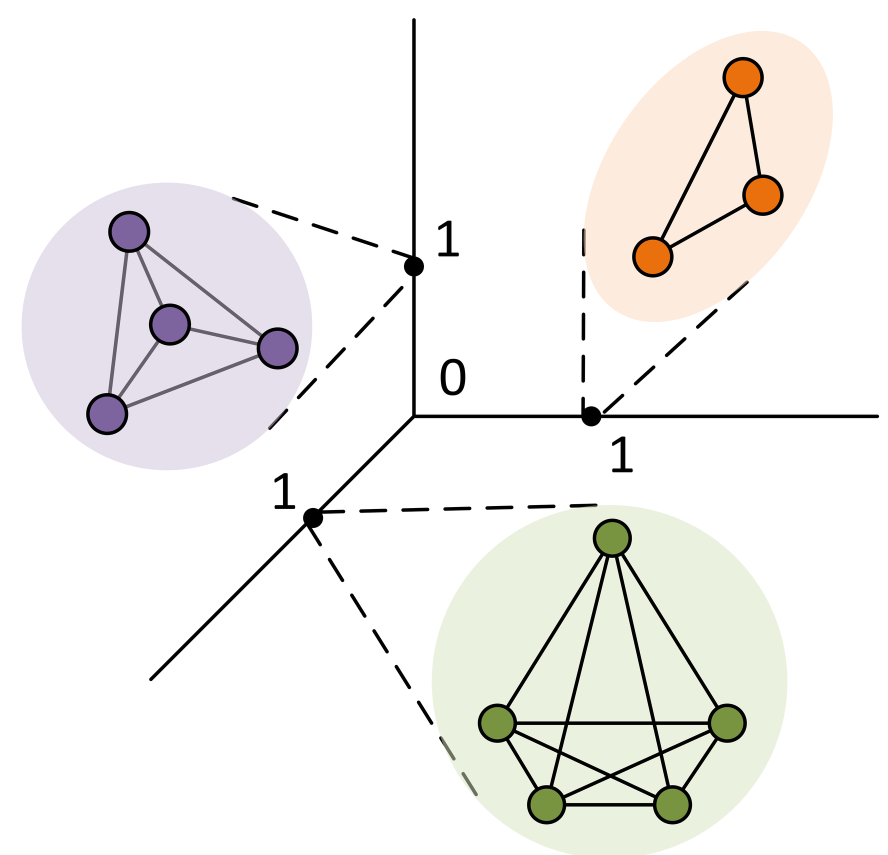

Figure 2: Lovasz embeddings for a graph consisting of set cliques are mapped orthogonal dimensions.

Proposed Model

- We propose the use of Lovasz kernel in the conventional Graph Convolutional framework. The proposed model is as follows

$$f(\mathbf{X}, \mathbf{K}) = \mathrm{softmax}(\mathbf{K}\ \mathrm{ReLU}(\mathbf{K}\mathbf{X}\mathbf{W}^{(0)})\mathbf{W}^{(1)}),$$

where $\mathbf{K}$ is the Lovasz or KLS kernel.

- The model is trained using cross entropy loss function as follows.

$$\mathcal{L} = \sum_{l \in \mathcal{Y}_L} \sum_{f=1}^{F} Y_{lf} \ln Z_{lf}.$$

Experiments

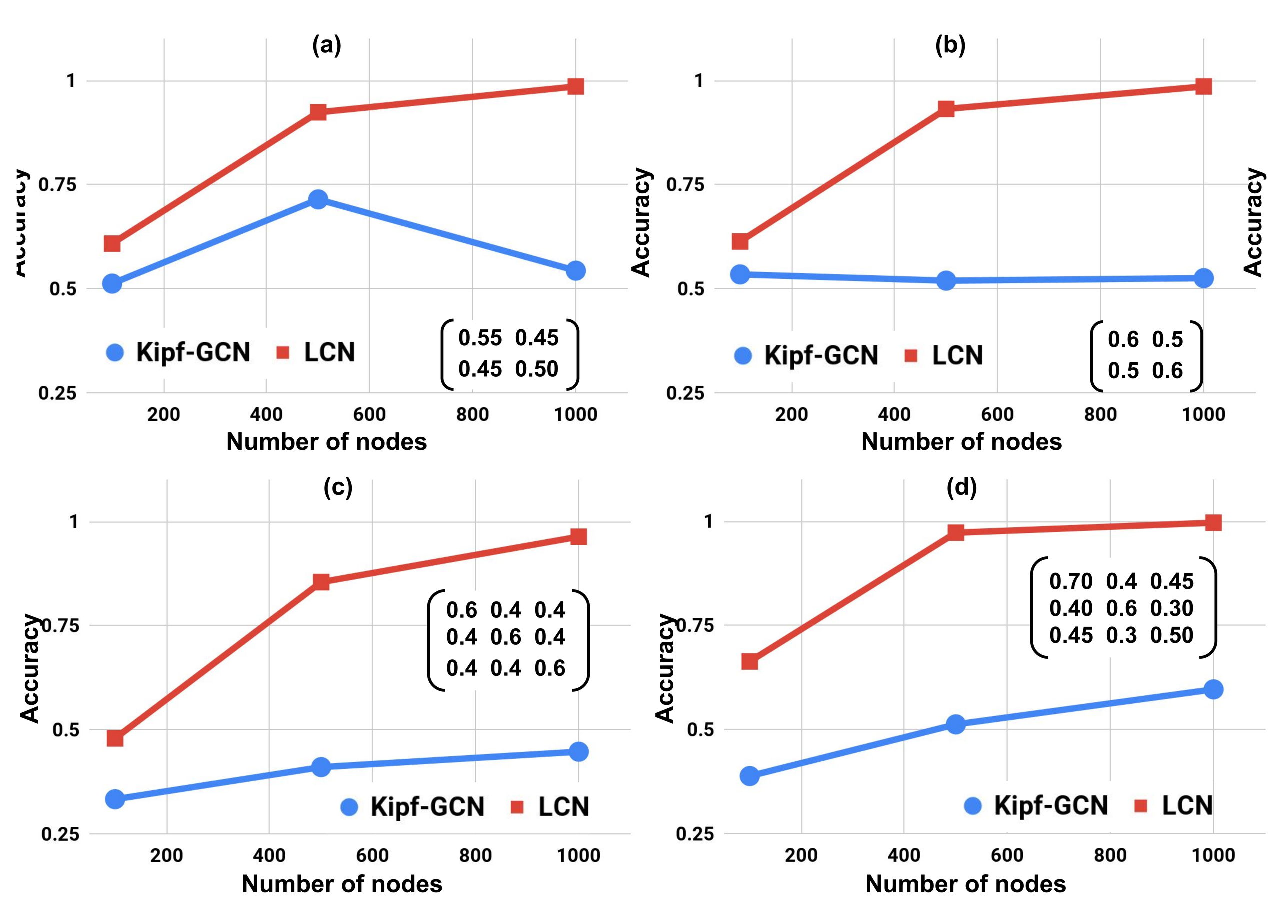

Figure 3: Test accuracy plots for various synthetically generated graphs from stochastic block model.

Experiments

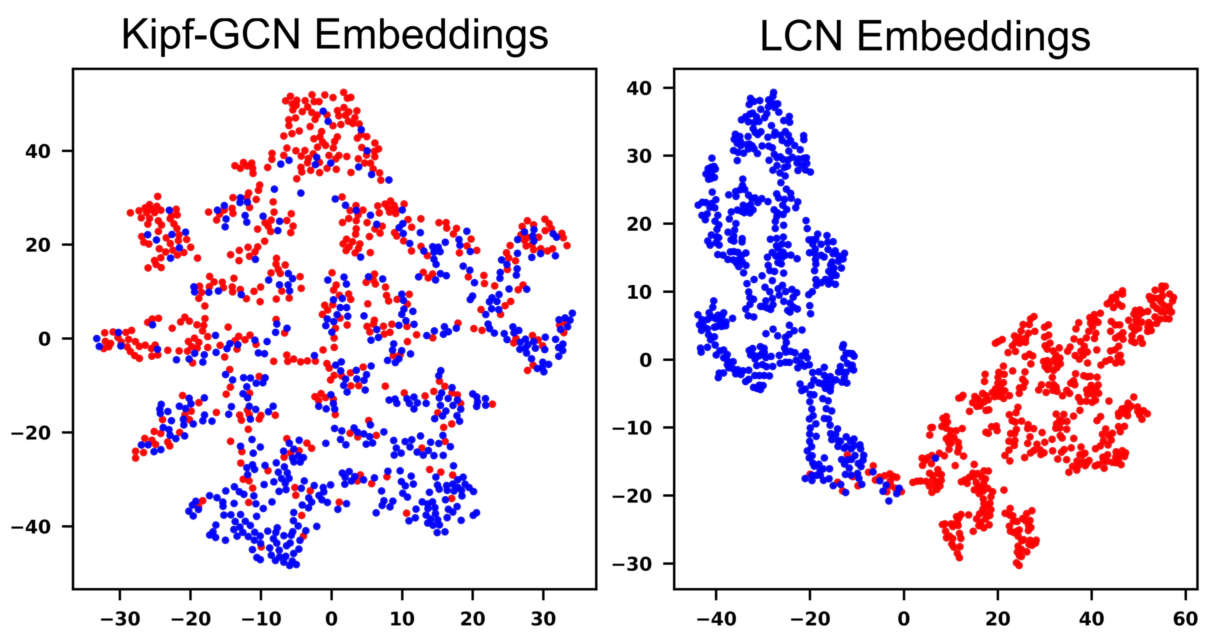

Figure 4: Embeddings learnt for settings corresponding to previous figure's (a) for n=1000

Dataset	Un-Lap	N-Lap	KS	SPORE	Kipf-GCN	GPNN	LCN
breast-cancer	88.2	93.3	92.8	96.7	**97.6**	95.5	97.2
diabetes	68.9	69.3	69.4	73.3	71.4	68.0	**76.3**
fourclass	70.0	70.0	70.4	78.0	80.5	73.9	**81.7**
heart	72.0	75.6	76.4	82.0	**85.1**	81.1	82.5
ionosphere	67.8	68.0	68.1	76.1	76.1	70.0	**87.9**
sonar	58.8	59.0	59.3	63.9	71.4	64.8	**73.2**
mnist-500 1 vs 2	75.6	80.6	79.7	85.8	98.0	96.2	**99.0**
mnist-500 3 vs 8	76.9	81.9	83.3	86.1	92.3	83.1	**93.7**
mnist-500 4 vs 9	68.4	72.0	72.2	74.9	**89.4**	88.5	83.3
mnist-2000 1 vs 2	83.8	96.2	95.0	96.7	99.0	97.5	**99.2**
mnist-2000 3 vs 8	55.2	87.4	87.4	91.4	94.7	89.6	**95.7**
mnist-2000 1 vs 7	90.7	96.8	96.6	97.3	**98.8**	96.4	98.7

Table 1: Binary Classification with Random label-to-color assignment in UCI and MNIST datasets.

Dataset	Node2vec	Kipf-GCN	GPNN	LCN
Citeseer	23.1	70.3	69.7	**73.5**
Cora	31.9	81.5	81.8	**82.6**
Pubmed	42.3	79	79.3	**79.7**

Table 2: Performance for SSL on Citeseer, Cora, Pubmed datasets

(n, k)	Kipf-GCN	LCN	Avg_same	Avg_diff
(50, 10)	0.92	**0.93**	0.83	-0.008
(75, 6)	0.77	**0.80**	0.80	-0.005
(100, 5)	0.71	**0.73**	0.79	-0.003
(100, 7)	**0.81**	**0.81**	0.80	-0.003

Table 3: Caveman graph experiment: Average test accuracy of Kipf-GCN and LCN on caveman graphs.

Figure 5: Behavior of test accuracy with increase in the heterogeneous edges in the hypergraph.

Source Code and Acknowledgement

- Codes: `https://github.com/malllabiisc/lcn/`.
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- This work was supported by MHRD, Govt. of India, and by gifts from Google Research and Accenture.