

Structural Neighborhood Based Classification of Nodes in a Network

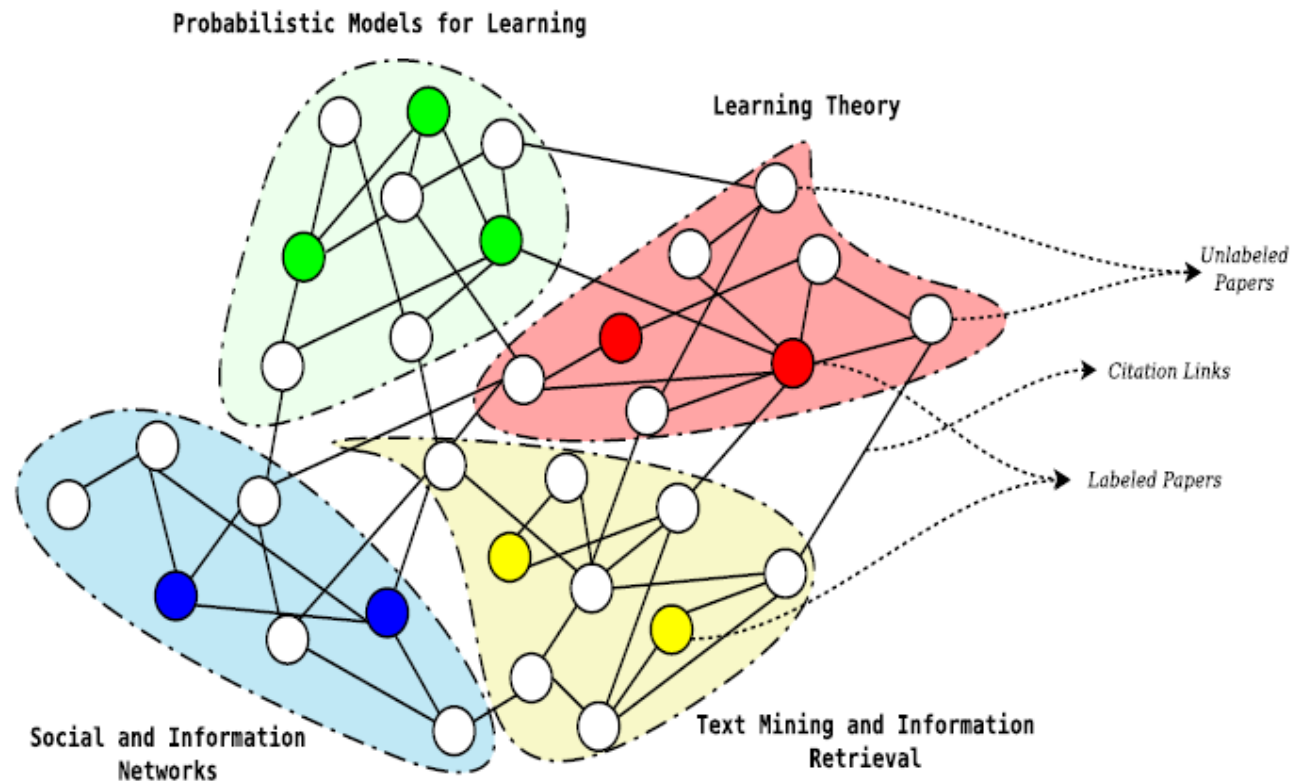
基于结构邻域的网络节点分类

KDD

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Purpose



- propose a novel structural neighborhood-based classifier learning using a random walk under sparse network

(1)

- homophily [1]: neighboring nodes in a network are supposed to be similar to each other.
- To exploit homophily in networks, we take a comprehensive view of classification, where a node is classified based on how other nodes in its extended neighborhood are labeled.

[1] A. Anagnostopoulos, R. Kumar, and M. Mahdian. Influence and correlation in social networks. In KDD, pages 7–15. ACM, 2008.

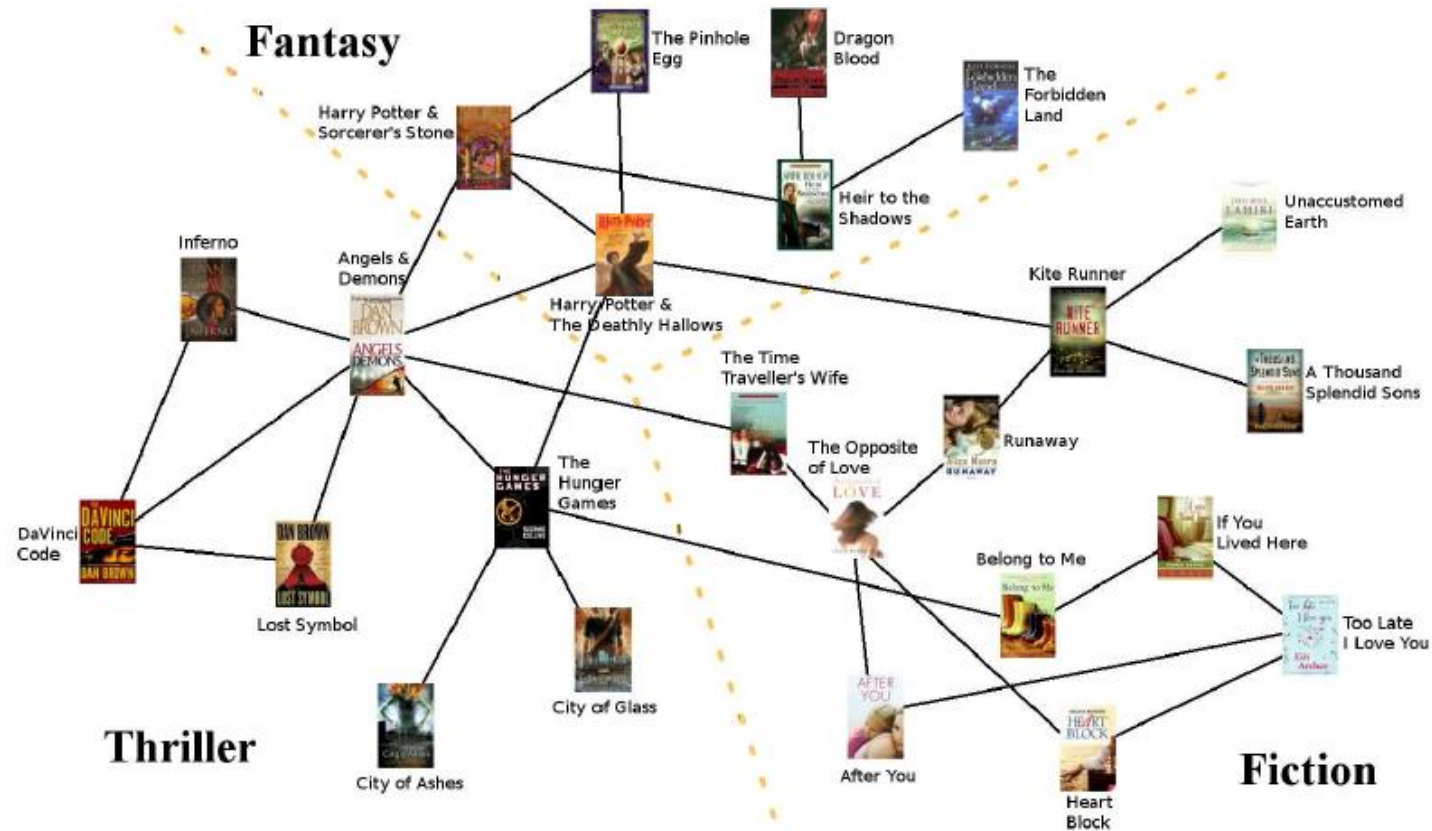
(2)

- A simple approach: use the number of neighbors from the respective classes and label the node based on majority voting.
- However, if the network is sparse, it did not work well. The label is sparse too.
- Propose a method: **weight vote instead of count**



What affect weight ?

S. A. Macskassy and F. Provost. A simple relational classifier. In MRDM at KDD, 2003.



- It is observed that high degree nodes are generally the source of linkage noise in networks.

- They think should a link to a low or medium degree node should be considered more reliable

- So ! ! ! Degree could affect the weight

Some Prepared

- In this paper, we will be working with a binary classification problem
- Let C^+ and C^- represent the sets of positive and negative examples respectively in the binary classification problem under consideration.

DEFINITION 1. *A network is modeled as a graph $\mathcal{G}(\mathcal{V}, \mathcal{E}, \mathcal{W})$, where \mathcal{V} is the set of $|\mathcal{V}| = n$ interacting units (nodes or actors), and $\mathcal{E} \subseteq \mathcal{V} \times \mathcal{V}$ is the set of edges indicating relationship or interactions among the nodes. $\mathcal{W} \in \mathbb{R}^{n \times n}$, where \mathcal{W}_{ij} indicates affinity or strength of the relationship between nodes $v_i, v_j \in \mathcal{V}$.*

For a sparsely labeled network, the classification problem is formally stated as follows.

DEFINITION 2. *Given a graph $\mathcal{G}(\mathcal{V}, \mathcal{E})$ and a set of labeled nodes \mathcal{V}_l ($\subsetneq \mathcal{V}$) with corresponding (ordered) set of labels $\mathcal{Y}_l \in \mathcal{C}^{|\mathcal{V}_l|}$, where $\mathcal{C} = \{\mathcal{C}_1, \mathcal{C}_2, \dots, \mathcal{C}_k\}$, the set of k labels \mathcal{C}_1 to \mathcal{C}_k . The objective is to learn a model for inferring labels of the unlabeled nodes $\mathcal{V}_u = \mathcal{V} \setminus \mathcal{V}_l$.*

We start by defining the adjacency based representation of a graph. Given an undirected and binary-weighted graph $\mathcal{G}(\mathcal{V}, \mathcal{E})$, where $\mathcal{V} = \{v_1, v_2, \dots, v_n\}$ and $\mathcal{E} \subseteq \mathcal{V} \times \mathcal{V}$, the corresponding adjacency matrix A is defined as follows,

$$A_{ij} = \begin{cases} 1, & \text{if } (v_i, v_j) \in \mathcal{E} \\ 0, & \text{otherwise} \end{cases}.$$

In the case of a weighted graph $\mathcal{G}(\mathcal{V}, \mathcal{E}, \mathcal{W})$, links carry a non-negative weight specified by \mathcal{W} . Adjacency Matrix A for these graphs is modified as $A_{ij} = \mathcal{W}_{ij}$. Based on the link attributes of a node, we define node v_i in vector space notation as $a_i = [A_{ji}]_{n \times 1}$ where $j \in \{1, 2, \dots, n\}$.

DEFINITION 3. *First-Level Neighborhood* of a node v_i is the set \mathcal{N}_i^1 s.t. $v_j \in \mathcal{N}_i^1$ if and only if there exists an edge in the graph connecting v_i and v_j , i.e., $(v_i, v_j) \in \mathcal{E}$.

the follow problem



约束最优化问题

$$\min_{w,b} \quad \frac{\lambda}{2} \|p\|^2 + \frac{1}{|\mathcal{V}_l|} \sum_{i \in \mathcal{V}_l} \varepsilon_i \quad (2)$$

such that $y_i(w^\top m_i + b) \geq 1 - \varepsilon_i$,
 $\varepsilon_i \geq 0$, and
 $m_i = A \frac{a_i}{d_i}$

(1) Structural Neighborhood: For a node v_i having class label $y_i \in \{-1, 1\}$, the aggregated scores from the nodes having label y_i in the first-level neighborhood (\mathcal{N}_i^1) should be more than the aggregated scores from rest of the nodes in the first-level neighborhood. Thus, for optimal w and b , we have, for all i ,

$$y_i \sum_{j \in \mathcal{N}_{i, y_i}^1} A(v_i, v_j)(w^\top \cdot a_j + b) \geq -y_i \sum_{j \in \mathcal{N}_{i, -y_i}^1} A(v_i, v_j)(w^\top \cdot a_j + b),$$

where $A(v_i, v_j) = A_{ij}$ indicates the weight of edge joining nodes v_i and v_j . This can be equivalently rewritten as,

$$y_i \left(\sum_{j \in \mathcal{N}_{i, y_i}^1} A_{ij}(w^\top \cdot a_j + b) + \sum_{j \in \mathcal{N}_{i, -y_i}^1} A_{ij}(w^\top \cdot a_j + b) \right) \geq 0,$$

$$\implies y_i \left(\sum_{j \in \mathcal{V}} A_{ij}(w^\top \cdot a_j + b) \right) \geq 0.$$

Rearranging the terms, we get,

$$y_i \left(w^\top \cdot A \cdot a_i + d_i b \right) \geq 0,$$

where $d_i = \sum_{j \in \mathcal{V}} A_{ij}$.

$$\implies y_i \left(\frac{1}{d_i} w^\top \cdot A \cdot a_i + b \right) \geq 0$$

$$r_i = y_i (w \cdot x_i + b)$$

Let $M = [m_1, m_2, \dots, m_n] = A^2 D^{-1}$, where $D \in \mathbb{R}^{n \times n}$ defined as $D_{ij} = \begin{cases} d_i & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$.

Then, we have the following in a linearly separable case:

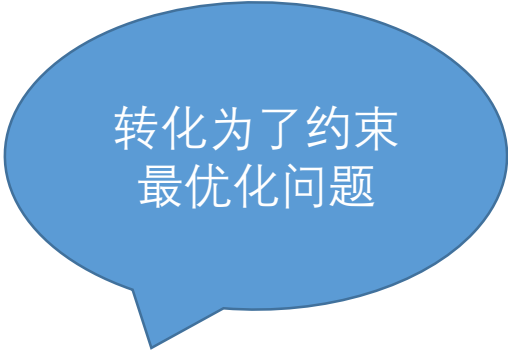
$$y_i(w^\top m_i + b) \geq 0.$$

The above can be interpreted as mapping the adjacency information a_i to a new space as $m_i = A \frac{a_i}{d_i}$, and then learning a decision boundary. For node v_i , we define empirical loss $\varepsilon_i (\geq 0)$ such that

$$y_i(w^\top m_i + b) \geq 1 - \varepsilon_i.$$

Mean empirical loss, that is to be minimized, is given by

$$f(w, b) = \frac{1}{|\mathcal{V}_l|} \sum_{i \in \mathcal{V}_l} \varepsilon_i. \quad (1)$$



转化为了约束最优化问题

Degree Dependent Regularization

- W depends on degree
- Add Degree Dependent Regularization p
- $p = (p_1, p_2, \dots, p_n)$ 其中 penalty for node v_i is $p_i = g(w_i, d_i)$.

- Linear Weighted Degree (**LWD**):

$$g(w_i, d_i) := |w_i| d_i$$

- Linear Weighted Root Degree (**LWRD**):

$$g(w_i, d_i) := |w_i| \sqrt{d_i}$$

- Linear Weighted Root Log Degree (**LWRLD**):

$$g(w_i, d_i) := |w_i| \sqrt{\log_2 d_i}$$

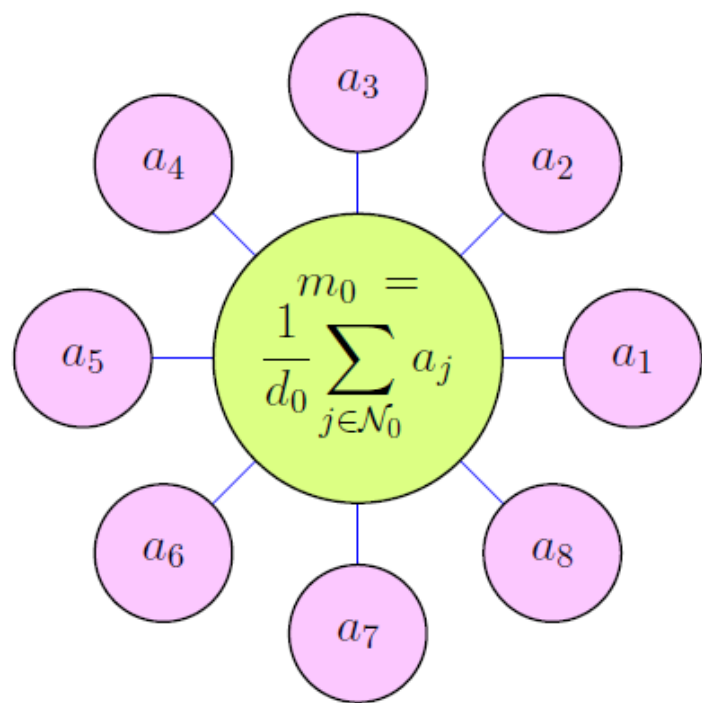
The objective function

Add a parameter λ

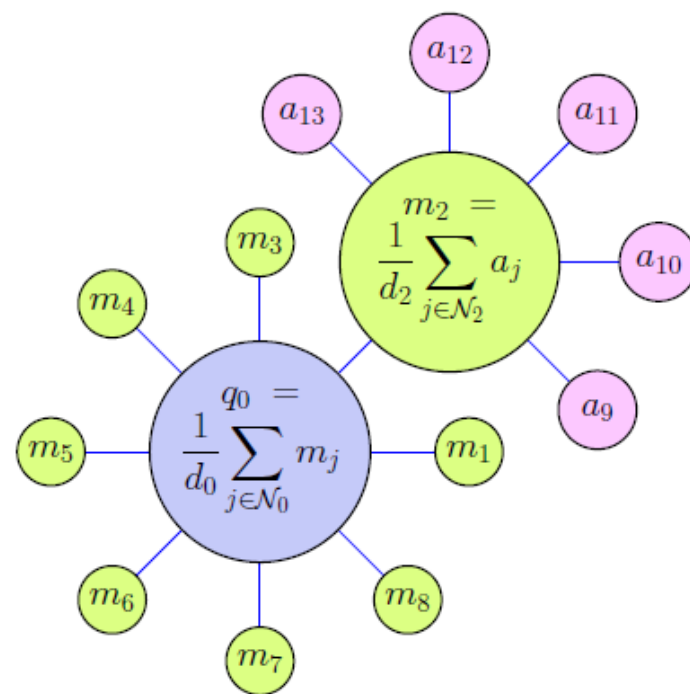
$$\min_{w,b} \quad \frac{\lambda}{2} \|p\|^2 + \frac{1}{|\mathcal{V}_l|} \sum_{i \in \mathcal{V}_l} \varepsilon_i \quad (2)$$

such that $y_i(w^\top m_i + b) \geq 1 - \varepsilon_i$,
 $\varepsilon_i \geq 0$, and
 $m_i = A \frac{a_i}{d_i}$

DEFINITION 4. r^{th} -**Level Neighborhood** of a node v_i is defined as a multiset \mathcal{N}_i^r s.t. $v_k \in \mathcal{N}_i^r$ if and only if there is an edge in graph \mathcal{G} connecting nodes v_k and v_j where node $v_j \in \mathcal{N}_i^{r-1}$, and multiplicity of v_k in \mathcal{N}_i^r is given by the cardinality of set $\{v_j | (v_k, v_j) \in \mathcal{E} \text{ and } v_j \in \mathcal{N}_i^{r-1}\}$.



(a) First-Level Neighborhood



(b) Second-Level Neighborhood

$$y_i \left(\sum_{j \in \mathcal{N}_{i, y_i}^1} A_{ij}(w^\top \cdot m_j + b) + \sum_{j \in \mathcal{N}_{i, -y_i}^1} A_{ij}(w^\top \cdot m_j + b) \right) \geq 0, \quad \forall i = 1, \dots, n$$

$$y_i \left(\frac{1}{d_i} w^\top \cdot A \cdot m_i + b \right) \geq 0, \quad \forall i = 1, \dots, n$$

where, $d_i = \sum_{j \in \mathcal{V}} A_{ij}$.

Let $Q = [q_1, q_2, \dots, q_n] = MAD^{-1} = A(AD^{-1})^2$, where M and D are defined in section [3](#). Then, for the linearly separable case, we have,

$$y_i(w^\top q_i + b) \geq 0, \quad \forall i = 1, \dots, n$$

where $q_i = A^2 D^{-1} \frac{a_i}{d_i}$ based on second-level neighborhood of a node. We can argue using inductive logic that while using r -level neighbors, the same will be mapped to $A(AD^{-1})^{r-1} \frac{a_i}{d_i}$.

For classification using r -level neighbors, the adjacency information contained in the matrix A as a whole gets mapped to $A(AD^{-1})^r$.

How to Random Walk

- Random Walk :

with increasing values of r , the transition probabilities between any pair of nodes start **converging towards the stationary probability distribution**.

- Lazy Random Walk:

- (1) length is not fixed.
- (2) Use dampening factor at each hop, which controls the termination of the random walk

- If dampening factor is γ , the random walk terminates at each hop with probability γ , and the next hop with probability $1-\gamma$. The representation obtained using the above process is given by

if γ is chosen to be close to zero, it is equivalent to learning with the given adjacency representation alone.

On the other extreme, if gamma is large (≈ 1), the same as random walk

$$q_i = (1-\gamma)A\left(e_i + \gamma \frac{a_i}{d_i} + \gamma^2 (AD^{-1}) \frac{a_i}{d_i} + \gamma^3 (AD^{-1})^2 \frac{a_i}{d_i} + \dots\right)$$

e_i being a n -dimensional unit vector with i^{th} entry as 1 and remaining as zeros.

Structured RandomWalk

- higher degree implies a higher termination probability and a lesser dampening factor

$$\gamma_i = \frac{1}{\log_2 d_i}.$$

We define matrix Γ as,

$$\Gamma = \text{diag}(\gamma_1, \gamma_2, \dots, \gamma_{|V|}).$$

The representation then becomes

$$q_i = A \left(e_i + \Gamma \frac{a_i}{d_i} + (AD^{-1}) \Gamma^2 \frac{a_i}{d_i} + (AD^{-1})^2 \Gamma^3 \frac{a_i}{d_i} + \dots \right) (I - \Gamma).$$

Let Q be the matrix obtained by stacking column vectors q_i corresponding to all the nodes. Then, we have

$$Q = A(I - AD^{-1}\Gamma)^{-1}(I - \Gamma).$$

The core of Algorithm

Taking structured random walk into account the objective in (2) is modified as:

$$\min_{w,b} \quad \frac{\lambda}{2} \|p\|^2 + \frac{1}{|\mathcal{V}_l|} \sum_{i \in \mathcal{V}_l} \varepsilon_i \quad (4)$$

$$\text{s.t.} \quad y_i(w^\top q_i + b) \geq 1 - \varepsilon_i, \\ \varepsilon_i \geq 0, \text{ and}$$

$$q_i = A \left(e_i + \Gamma \frac{a_i}{d_i} + (AD^{-1}) \Gamma^2 \frac{a_i}{d_i} + (AD^{-1})^2 \Gamma^3 \frac{a_i}{d_i} + \dots \right) (I - \Gamma)$$

Subgradient of the above is given by,

$$\nabla_t = \lambda p \frac{\partial p}{\partial w} - \frac{1}{|\mathcal{V}_l|} \sum_{i \in \mathcal{V}_l} \mathbb{1}[y_i w_t^\top q_i < 1] y_i q_i,$$

where $\mathbb{1}$ denotes indicator function. Using gradient descent, the iterative update rule for w is given by

$$w_{t+1} = w_t - \eta_t \nabla_t$$

where η_t is the learning rate for the t^{th} iteration. We use stochastic gradient descent mini-batch update algorithm with a variable learning rate η_t given by $\eta_t = \frac{1}{2 + \lambda t}$.

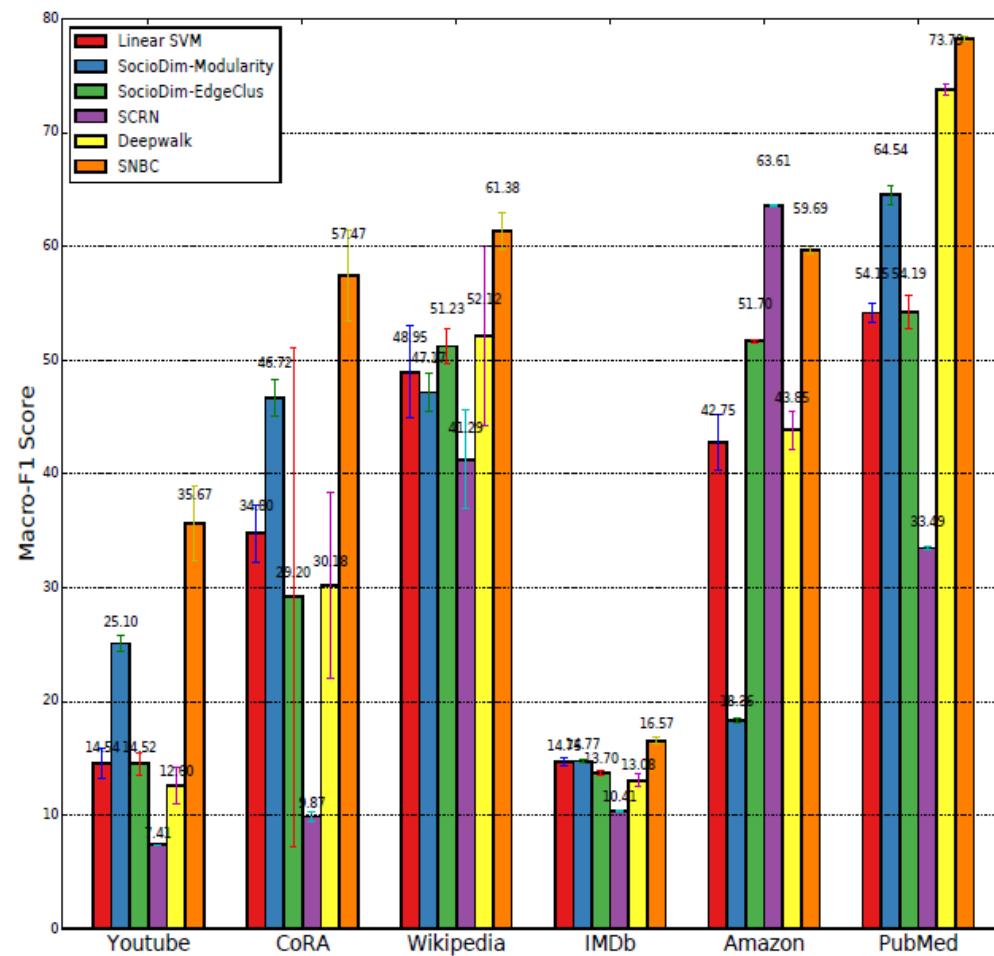
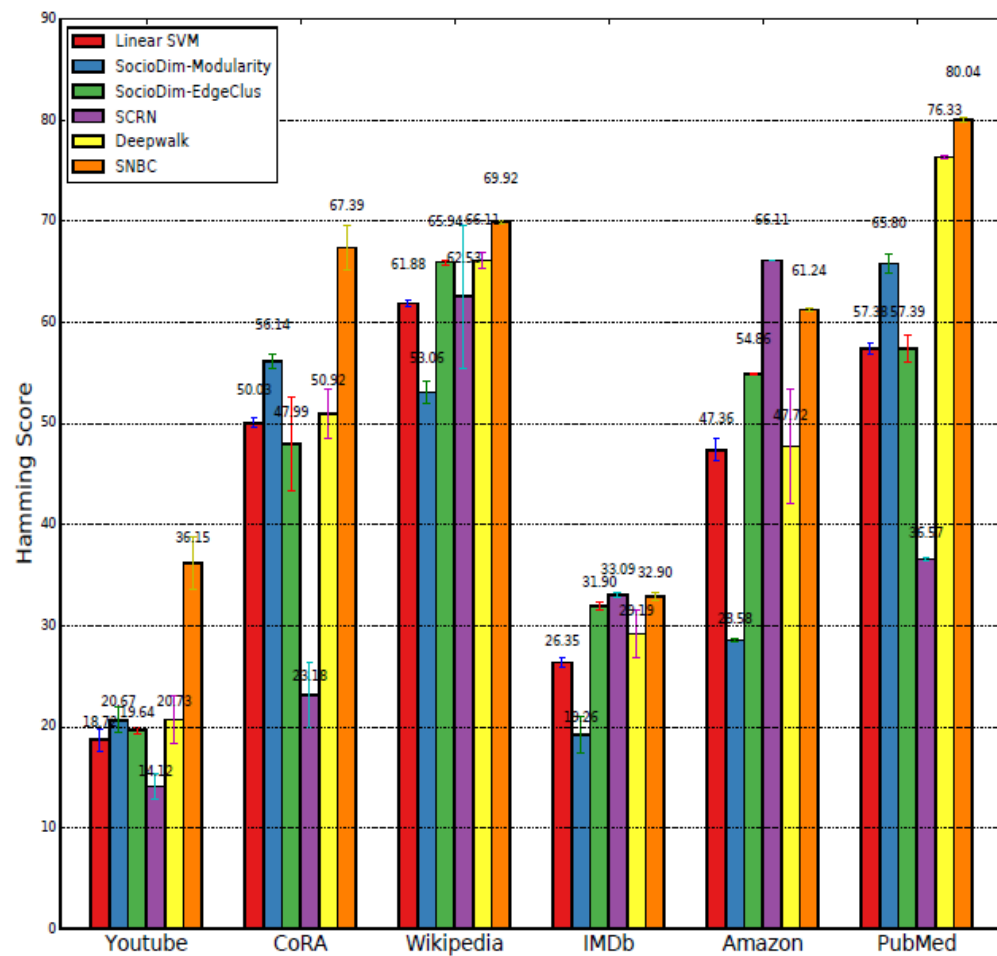
Experiment

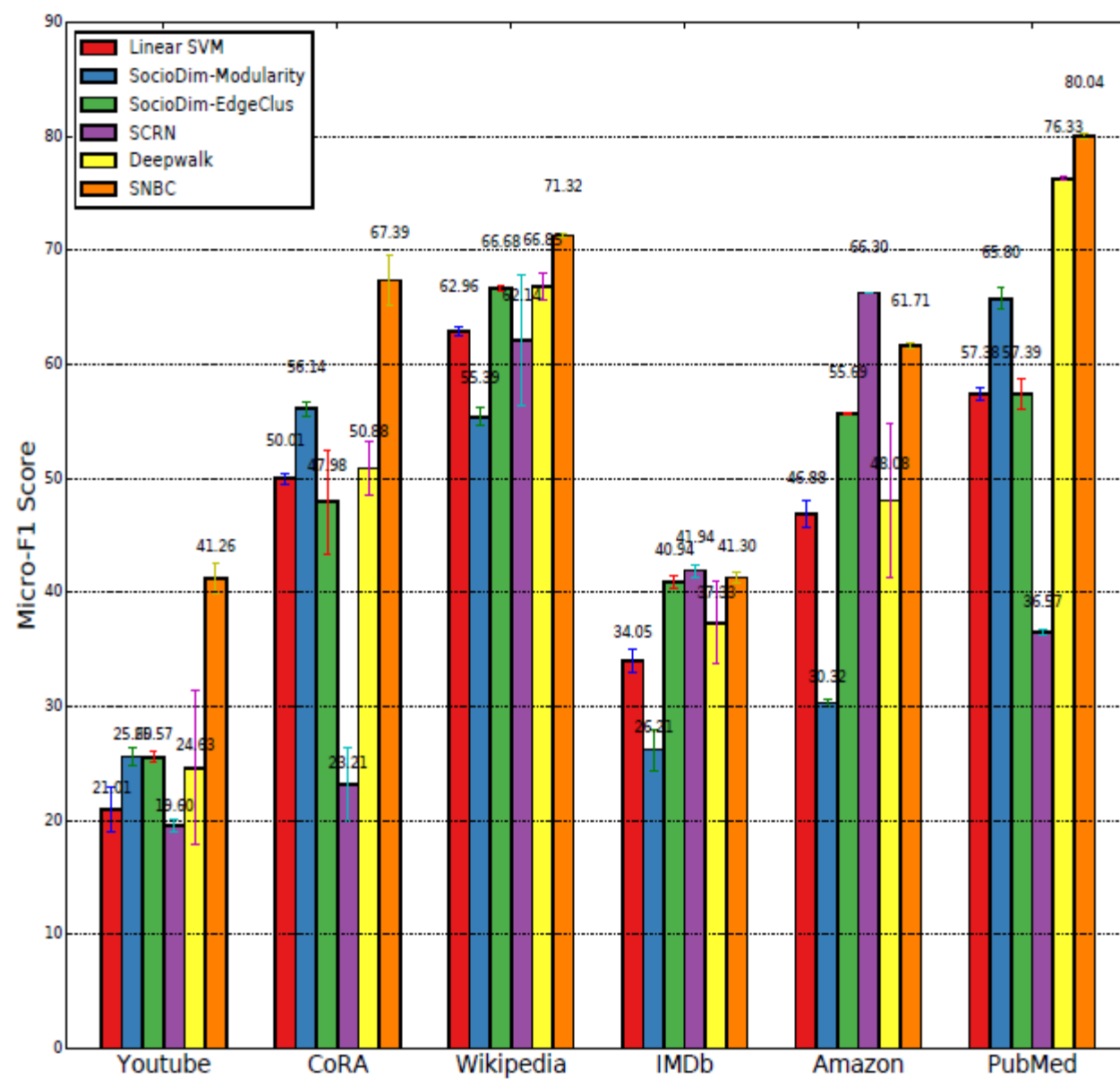
If for the i_{th} node, T_i is the set of true labels, and P_i is set of predicted labels

$$\text{Hamming Score} = \sum_i \frac{|T_i \cap P_i|}{|T_i \cup P_i|}$$

$$\text{Micro-}F_1 \text{ Score} = \frac{2 \sum_i |T_i \cap P_i|}{\sum_i |T_i| + \sum_i |P_i|}$$

$$\text{Macro-}F_1 \text{ Score} = \frac{1}{k} \sum_{j=1}^k \frac{2 \sum_{i \in \mathcal{C}_j} |T_i \cap P_i|}{\sum_{i \in \mathcal{C}_j} |T_i| + \sum_{i \in \mathcal{C}_j} |P_i|}$$





Thank you !