

# Learning from Labeled and Unlabeled Vertices in Networks

## 网络中标记和未标记顶点的学习

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*Definition 3.1. Geometric One-hop Neighborhood.* The geometric one-hop neighbors of a vertex  $v_i$  is defined as a set  $\mathcal{N}_i^1$  which contains those vertex  $v_j$  which can be reached by a random walker from  $v_i$  in one step. The geometric one-hop neighborhood is defined as a set  $\mathcal{N}^1 = \bigcup_{i=1}^l \mathcal{N}_i^1$ .

*Definition 3.2. Geometric  $m$ -hop Neighborhood.* The geometric  $m$ -hop neighbors of a vertex  $v_i$  is defined as a set  $\mathcal{N}_i^m$  which contains those vertex  $v_j$  which can be reached by a random walker from  $v_i$  in  $m$  steps. The geometric  $m$ -hop neighborhood is defined as a set  $\mathcal{N}^m = \bigcup_{i=1}^l \mathcal{N}_i^m$ .

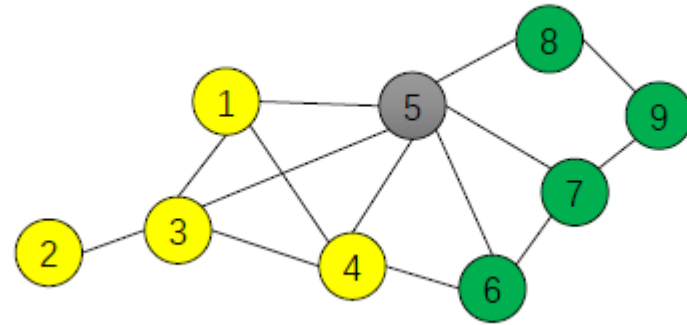
The affinity matrix of vertices is denoted by  $A \in \mathbb{R}^{n \times n}$  with  $a_{i,j} = a_{j,i}, a_{i,i} = 0$ . The degree matrix  $D$  is a diagonal matrix associated with  $A$  with  $d_{i,i} = \sum_j a_{j,i}$ . The random walk transition matrix  $P$  is defined as  $D^{-1}A$ .

We denote a vertex  $v_q$  in the geometric one-hop neighborhood  $N^1$  by  $p_q$  which is the  $q^{th}$  row of the transition matrix  $P$ .

$$f(p_q) = p_q \cdot w^\top + b \quad (1)$$

$$y_q = \text{sign}(f(p_q)) = \text{sign}(p_q \cdot w^\top + b) \quad (2)$$

Equation (1) does not take the neighborhood relationship into consideration to classify vertices in networks, which would lead to the deterioration of the classifier.



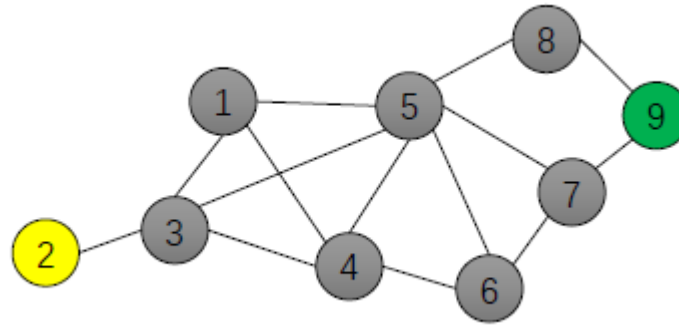
what is the label of the  
vertex v5?

use a weighted-vote strategy

$$\begin{aligned} f(\mathbf{p}_q) &= \mathbf{p}_q \cdot \mathbf{w}^\top + b > 0 \\ y_q &= 1 \\ \text{if } \frac{\sum_{i \in \mathcal{N}_q^1} a_{i,q} f(\mathbf{p}_i)}{\sum_{i \in \mathcal{N}_q^1} a_{i,q}} &\geq +1 \end{aligned} \quad (3)$$

$$\begin{aligned} f(\mathbf{p}_q) &= \mathbf{p}_q \cdot \mathbf{w}^\top + b < 0 \\ y_q &= -1 \\ \text{if } \frac{\sum_{i \in \mathcal{N}_q^1} a_{i,q} f(\mathbf{p}_i)}{\sum_{i \in \mathcal{N}_q^1} a_{i,q}} &\leq -1 \end{aligned} \quad (4)$$

$$\begin{aligned} y_q \cdot \frac{\sum_{i \in \mathcal{N}_q^1} a_{i,q} (\mathbf{p}_i \cdot \mathbf{w}^\top + b)}{\sum_{i \in \mathcal{N}_q^1} a_{i,q}} &\geq 1 \\ \Rightarrow y_q \cdot \left( \frac{\sum_{i \in \mathcal{N}_q^1} a_{i,q} \cdot \mathbf{p}_i}{d_{q,q}} \cdot \mathbf{w}^\top + b \right) &\geq 1 \\ \Rightarrow y_q \cdot \left( \frac{\mathbf{a}_q \cdot \mathbf{P}}{d_{q,q}} \cdot \mathbf{w}^\top + b \right) &\geq 1 \\ \Rightarrow y_q \cdot (\mathbf{p}_q \cdot \mathbf{P} \cdot \mathbf{w}^\top + b) &\geq 1 \end{aligned} \quad (5)$$



what is the label of the  
vertex v5?

# Geometric m-hop Neighborhood

In the geometric  $m$ -hop neighborhood  $\mathcal{N}_i^m$ ,  $v_q$  is denoted by  $\mathbf{p}_q^m$  which is the  $q$ -th row of the transition matrix  $\mathbf{P}^m$ . If we replace  $\mathbf{p}_q$  in the Inequality (5) with  $\mathbf{p}_q^m$ , we have:

$$\begin{aligned} & y_q \cdot \frac{\sum_{i \in \mathcal{N}_q^m} a_{i,q} (\mathbf{p}_i^m \cdot \mathbf{w}^\top + b)}{\sum_{i \in \mathcal{N}_q^m} a_{i,q}} \geq 1 \\ \Rightarrow & y_q \cdot \left( \frac{\sum_{i \in \mathcal{N}_q^m} a_{i,q} \cdot \mathbf{p}_i^m}{d_{q,q}} \cdot \mathbf{w}^\top + b \right) \geq 1 \\ \Rightarrow & y_q \cdot \left( \frac{\mathbf{a}_q \cdot \mathbf{P}^m}{d_{q,q}} \cdot \mathbf{w}^\top + b \right) \geq 1 \quad (6) \\ \Rightarrow & y_q \cdot (\mathbf{p}_q \cdot \mathbf{P}^m \cdot \mathbf{w}^\top + b) \geq 1 \\ \Rightarrow & y_q \cdot (\mathbf{p}_q^m \cdot \mathbf{P} \cdot \mathbf{w}^\top + b) \geq 1 \\ \Rightarrow & y_q \cdot (\mathbf{p}_q^{m+1} \cdot \mathbf{w}^\top + b) \geq 1 \end{aligned}$$

where  $\mathbf{p}_q^{m+1}$  is the representation of  $v_q$  in the geometric  $(m+1)$ -hop neighborhood.



$$\begin{aligned} y_q \cdot (\mathbf{p}_q^{m+1} \cdot \mathbf{w}^\top + b) &\geq 1 - \xi_q \\ \xi_q &\geq 0, \quad 1 \leq q \leq l, \quad m \geq 1 \end{aligned} \quad (7)$$

Similar to SVM, add a slack variable

# Unconstrained SVM problem

$$\min_{\mathbf{w}, b} \frac{1}{2} \mathbf{w} \cdot \mathbf{w}^\top + \frac{\alpha}{l} \sum_{q=1}^l \max(1 - y_q \cdot f(\mathbf{x}_q), 0)^2 \quad (8)$$

represent the vertex  $v_q$  by  $\mathbf{x}_q = \mathbf{p}_q^2 + \dots + \mathbf{p}_q^{m+1} = \mathbf{p}_q \cdot (\mathbf{P} + \dots + \mathbf{P}^m)$ .

$$\min_{\mathbf{w}} F(\mathbf{w}) = \frac{\lambda}{2} (\mathbf{w} \odot \mathbf{d})(\mathbf{w} \odot \mathbf{d})^\top + \frac{\alpha}{l} \sum_{q=1}^l \max(1 - y_q \mathbf{x}_q \mathbf{w}^\top, 0)^2 \quad (9)$$

$\mathbf{x}_q$  as  $[\mathbf{x}_q, 1]$  and  $\mathbf{w}$  as  $[\mathbf{w}, b]$ .

a damping factor at each hop

the  $m^{th}$  hop is defined as  $\rho^m / m!$ ,

$$\mathbf{x}_q = \left[ \mathbf{p}_q \cdot \left( \frac{\rho^1}{1!} \mathbf{P} + \dots + \frac{\rho^m}{m!} \mathbf{P}^m \right), 1 \right],$$

$$\mathbf{d} = \left[ \text{diag}(\mathbf{D}^{-\frac{1}{2}})^\top, 1 \right]$$

$\odot$  means the Hadamard product,

# How to jump out local optima ? (GCD)

- 1.GD(Gradient Decent)
- 2.CD(Coordinate Decent)
- What is Coordinate Decent?

- For  $f(x)$ ,  $\mathbf{x}^{(k-1)} \rightarrow \mathbf{x}^{(k)}$

$$x_1^{(k)} \in \operatorname{argmin}_{x_1} f(x_1, x_2^{(k-1)}, x_3^{(k-1)}, \dots, x_n^{(k-1)})$$

$$x_2^{(k)} \in \operatorname{argmin}_{x_2} f(x_1^{(k)}, x_2, x_3^{(k-1)}, \dots, x_n^{(k-1)})$$

$$x_3^{(k)} \in \operatorname{argmin}_{x_3} f(x_1^{(k)}, x_2^{(k)}, x_3, \dots, x_n^{(k-1)})$$

...

$$x_n^{(k)} \in \operatorname{argmin}_{x_n} f(x_1^{(k)}, x_2^{(k)}, x_3^{(k)}, \dots, x_n)$$

每一次我们解决了  $x_i^{(k)}$ ，我们都会使用新的值。

# GD

$$F'(\mathbf{w}) = \lambda \mathbf{w} \odot \mathbf{d} - \frac{2\alpha}{l} \sum_{j \in \mathbb{I}(\mathbf{w})} y_j \mathbf{x}_j b_j(\mathbf{w}) \quad (10)$$

where  $b_j(\mathbf{w}) = 1 - y_j \mathbf{x}_j \mathbf{w}^\top$  and  $\mathbb{I}(\mathbf{w}) = \{j | b_j(\mathbf{w}) > 0\}$ .

We iteratively update  $\mathbf{w}$  as follows:

$$\mathbf{w}^{t+1} = \mathbf{w}^t - \eta_t F'(\mathbf{w}^t) \quad (11)$$

where  $\eta_t$  is the learning rate at the  $t^{th}$  iteration and is chosen from  $\{1, \beta, \beta^2, \dots\}$  by a line search.

The last  $\mathbf{w}$  in GD is the first  $\mathbf{w}$  in CD


# CD

sequence  $\{\mathbf{w}^t\}$  ( $t = 0, 1, 2, \dots$ ). At each iteration,  $\mathbf{w}^{t+1}$  is produced by sequentially updating each entry of  $\mathbf{w}^t$  with other entries fixed. The process produces a sequence of vectors  $\mathbf{w}^{t,i}$  ( $i = 1, \dots, n+1$ ), such that  $\mathbf{w}^{t,0} = \mathbf{w}^t$ ,  $\mathbf{w}^{t,n+1} = \mathbf{w}^{t+1}$  and

$$\mathbf{w}^{t,i} = [w_1^{t+1}, \dots, w_i^{t+1}, w_{i+1}^t, \dots, w_{n+1}^t]$$

Updating  $\mathbf{w}^{t,i}$  to  $\mathbf{w}^{t,i+1}$  becomes the following one-variable sub-problem:

$$\begin{aligned}
 & \min_z F_i(\mathbf{w}_1^{t+1}, \dots, \mathbf{w}_i^{t+1}, \mathbf{w}_{i+1}^t + z, \mathbf{w}_{i+2}^t, \dots, \mathbf{w}_{n+1}^t) \\
 & \equiv \min_z F_i(\mathbf{w}^{t,i} + z\mathbf{e}_i) \\
 & = \min_z \frac{\lambda}{2} \left( (\mathbf{w}^{t,i} + z\mathbf{e}_i) \odot \mathbf{d} \right) \left( (\mathbf{w}^{t,i} + z\mathbf{e}_i) \odot \mathbf{d} \right)^\top \quad (12) \\
 & \quad + \frac{\alpha}{l} \sum_{j \in \mathbb{I}(\mathbf{w}^{t,i} + z\mathbf{e}_i)} (b_j(\mathbf{w}^{t,i} + z\mathbf{e}_i))^2
 \end{aligned}$$

where  $\mathbf{e}_i \in \mathbb{R}^{1 \times (n+1)}$  is a vector with the  $i^{th}$  entry 1 and all other entries 0. 

The first derivative of (12) with respect to  $z$  is:

$$F'_i(z) = \lambda \left( \mathbf{w}_i^{t,i} + z \right) \cdot \mathbf{d}_i - \frac{2\alpha}{l} \sum_{j \in \mathbb{I}(\mathbf{w}_i^{t,i} + z\mathbf{e}_i)} (y_j x_{j,i} (b_j(\mathbf{w}_i^{t,i} + z\mathbf{e}_i))) \quad (13)$$

As pointed out in [4],  $F_i(z)$  is not twice differentiable at some  $j$ , where  $b_j(\mathbf{w}_i^{t,i} + z\mathbf{e}_i) = 0$ . Following [4, 19], we define the generalized second derivative of (12) with respect to  $z$  as:

$$F''_i(z) = \lambda \mathbf{d}_i + \frac{2\alpha}{l} \sum_{j \in \mathbb{I}(\mathbf{w}_i^{t,i} + z\mathbf{e}_i)} x_{j,i}^2 \quad (14)$$

The Newton direction at a given  $z$  is  $\frac{F'_i(z)}{F''_i(z)}$ . We start from  $z = 0$  and apply a line search  $z = z - \eta_i \frac{F'_i(z)}{F''_i(z)}$  until  $F_i(z - \eta_i \frac{F'_i(z)}{F''_i(z)}) < F_i(z)$ , where  $\eta_i$  is the learning rate for the  $i^{th}$  element and is chosen from  $\{1, \beta, \beta^2, \dots\}$ .

[4] Kai-Wei Chang, Cho-Jui Hsieh, and Chih-Jen Lin. 2008. Coordinate descent method for large-scale l2-loss linear support vector machines. *Journal of Machine Learning Research* 9, Jul (2008), 1369–1398.

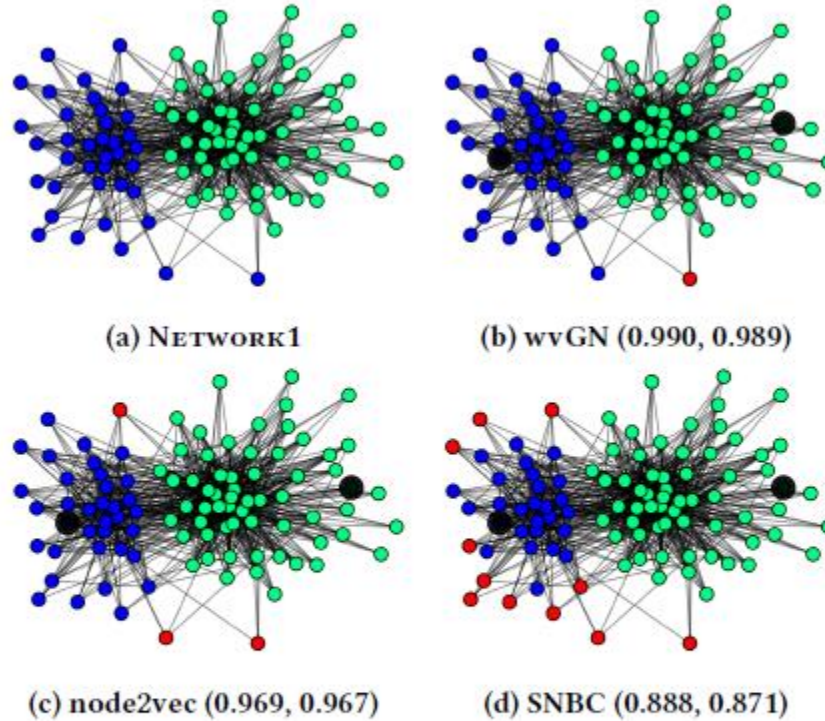
# Complexity analysis.

- Assume that a network has  $n$  vertices and  $r$  edges,  $l$  is the number of the labeled vertices,  $k$  is the number of  $w$  elements.

$$O(n \cdot (r + k \cdot l)).$$

# Experiment

- Network1 has 100 into two classes (3 is 21).



are grouped  
) average degree

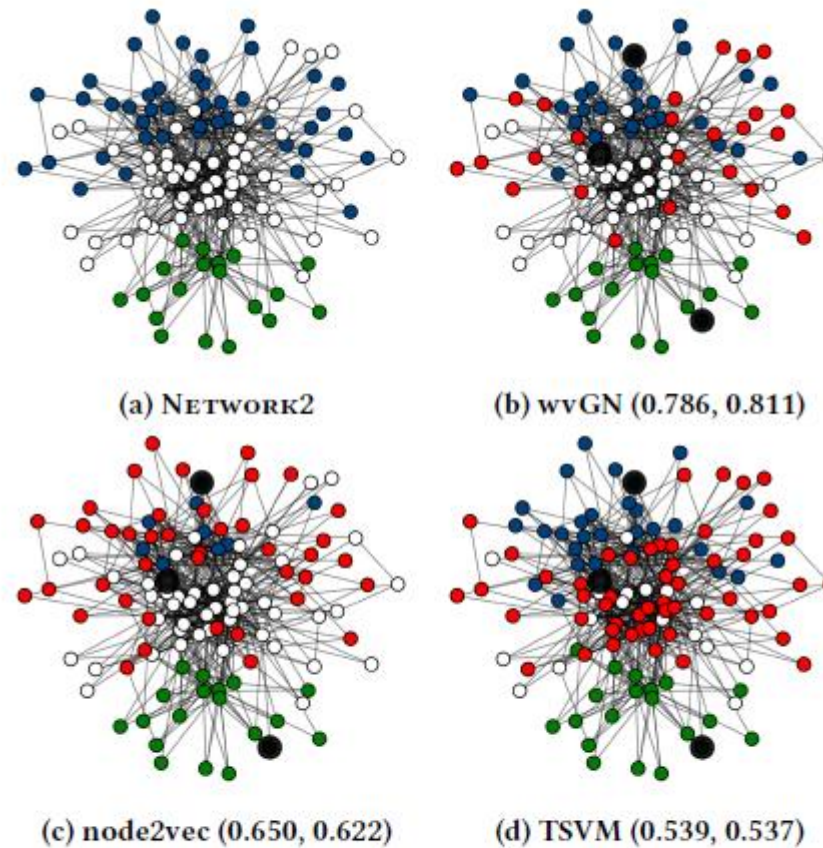
Figure 4: Classification results on NETWORK1. The two labeled vertices are in black and the misclassified vertices are in red. Subcaption: Method (Micro-F1, Macro-F1).



Table 1: Classification results on NETWORK1 with the varying number of labeled vertices (#LV) in each class.

#LV	Micro-F1 (%)					Macro-F1 (%)				
	1	2	3	4	5	1	2	3	4	5
wvGN	98.7±0.7	98.9±0.3	99.3±0.5	99.0±0.3	99.2±0.5	98.6±0.7	98.8±0.4	99.2±0.6	98.9±0.3	99.2±0.5
wvGN (full)	98.7±0.5	98.8±0.7	99.3±0.5	99.0±0.6	99.2±0.5	98.6±0.5	98.7±0.7	99.2±0.6	98.9±0.7	99.2±0.6
node2vec	96.9±0.5	94.5±6.0	94.8±5.1	94.5±5.6	94.2±5.4	96.7±0.5	94.3±5.9	94.6±5.1	94.2±5.5	94.0±5.4
Deepwalk	74.6±26.7	75.6±20.7	77.8±18.9	75.9±20.1	79.6±12.0	74.3±26.9	74.5±22.4	77.0±19.9	75.0±21.2	78.7±12.4
SNBC	85.6±15.6	81.2±17.4	71.4±10.7	71.3±10.5	74.9±10.3	84.0±16.6	80.9±17.8	70.9±10.8	70.5±10.6	73.8±10.0
wvRN	77.9±19.2	66.6±18.5	76.3±21.1	86.7±17.7	92.6±7.3	71.5±25.2	55.1±24.0	70.8±25.7	84.3±20.4	91.7±8.2
SCRN	77.3±22.4	74.2±21.8	81.2±17.2	86.3±13.6	90.2±10.6	66.6±32.3	61.0±31.8	73.5±25.6	80.6±21.5	87.0±16.2
SocDim	55.2±9.9	52.0±8.5	53.7±5.8	57.2±6.2	60.0±6.3	51.8±10.2	49.7±7.5	52.4±4.6	54.9±5.8	58.4±5.4
HeatKernel	82.4±19.8	68.8±20.0	78.6±21.2	88.2±16.3	90.9±11.9	77.7±25.9	57.9±26.1	73.8±25.8	86.6±18.0	90.2±12.3
LGC	60.4±18.6	55.6±18.3	60.5±21.9	62.1±22.1	62.4±17.0	45.1±22.4	39.5±19.7	47.5±26.4	46.9±27.0	45.1±20.1
TSVM	37.8±0	37.5±0	37.2±0	37.0±0	36.7±0	27.4±0	27.3±0	27.1±0	27.0±0	26.8±0
LapSVM	51.9±9.4	52.9±8.8	56.0±8.5	58.2±14.4	65.1±12.8	41.6±8.9	45.6±9.9	49.7±8.2	52.9±16.7	62.4±12.4

- Network2 has :  
three classes (1  
degree is 10.



rich are grouped into  
(relatively). average

Figure 5: Classification results on NETWORK2. The three labeled vertices are in black and the misclassified vertices are in red. Subcaption: Method (Micro-F1, Macro-F1).

Table 2: Classification results on NETWORK2 with the varying number of labeled vertices (#LV) in each class.

#LV	Micro-F1 (%)					Macro-F1 (%)				
	1	2	3	4	5	1	2	3	4	5
wvGN	66.7±11.4	71.8±11.0	<b>77.3±14.5</b>	<b>89.0±2.7</b>	<b>88.9±2.5</b>	67.7±12.2	73.3±11.6	<b>79.1±15.0</b>	<b>90.9±2.5</b>	<b>90.9±2.1</b>
wvGN (full)	<b>67.4±10.1</b>	<b>79.9±7.6</b>	69.6±15.8	86.3±3.5	84.1±5.8	<b>68.1±10.4</b>	<b>82.3±7.1</b>	71.4±15.1	87.7±4.2	85.3±6.0
node2vec	60.4±9.7	70.5±7.3	61.8±11.5	67.9±10.9	67.9±10.9	58.9±12.3	71.8±8.2	61.2±12.6	67.8±12.3	67.8±12.3
Deepwalk	42.4±7.4	46.5±7.1	42.9±12.6	51.2±5.9	51.2±5.9	40.7±7.2	45.2±6.8	41.7±11.7	48.5±5.8	48.5±5.8
SNBC	35.8±6.7	45.5±12.8	48.7±12.3	56.0±5.0	57.2±4.8	35.3±12.0	43.8±13.1	46.0±13.9	56.7±5.8	57.9±4.9
wvRN	45.0±12.1	56.0±15.7	56.9±11.3	68.1±7.5	68.1±7.5	36.2±13.9	49.4±17.8	53.9±14.9	64.8±11.6	64.8±11.6
SCRN	45.9±14.6	50.3±14.8	57.3±10.3	57.2±4.8	65.2±10.3	36.3±16.4	39.7±18.3	50.1±15.2	57.9±4.9	58.7±17.4
SocDim	31.0±7.9	37.0±7.6	42.9±7.2	44.5±4.7	44.5±4.7	29.1±6.7	35.4±6.5	41.3±6.7	42.1±5.2	42.1±5.2
HeatKernel	48.3±10.1	57.3±16.4	55.3±12.6	65.1±8.0	65.1±8.0	40.2±14.5	52.2±17.7	52.5±14.7	59.6±12.0	59.6±12.0
LGC	31.2±5.1	31.3±4.7	31.5±8.0	35.2±4.8	35.2±4.8	29.6±3.5	29.0±3.6	28.4±6.7	32.1±3.8	32.1±3.8
TSVM	54.2±5.0	64.6±7.5	51.7±4.1	52.0±4.9	52.0±4.9	53.5±5.0	64.7±6.7	51.4±4.1	51.7±4.9	51.7±4.9
LapSVM	37.6±13.2	49.4±10.7	58.3±10.5	63.1±8.5	63.1±8.5	23.4±8.6	39.1±11.2	56.9±12.3	66.0±7.9	66.0±7.9

- For the real-world data, we use four popular relational datasets
- CoRA, PubMed, IMDB, Wikipedia

Table 3: Classification results on CoRA (#vertices: 24,519, #edges: 92,207, #classes: 10) with the varying percent of labeled vertices (%LV). N/A means the results are not available because the algorithm is not finished in one week.

[illegible]

Table 4: Classification results on PUBMED (#vertices: 19,717, #edges: 44,324, #classes: 3) with the varying percent of labeled vertices (%LV).

[illegible]



Table 6: Classification on WIKIPEDIA (#vertices: 4,777, #edges: 184,812, #classes: 40) with the varying percent of labeled vertices (%LV).

%LV	Micro-F1 (%)					Macro-F1 (%)				
	1%	3%	5%	7%	9%	1%	3%	5%	7%	9%
wvGN	41.6±1.0	<b>45.3±0.6</b>	<b>44.9±1.0</b>	<b>45.4±1.0</b>	<b>45.4±0.7</b>	<b>6.5±0.4</b>	6.8±0.4	6.3±0.4	6.8±0.5	6.6±0.3
node2vec	29.3±5.0	31.2±1.8	31.1±2.4	31.7±2.6	34.3±4.2	6.4±0.4	<b>7.1±0.2</b>	<b>7.6±0.5</b>	<b>8.0±0.6</b>	<b>8.3±0.5</b>
deepwalk	17.7±1.5	14.0±1.2	13.5±1.4	13.8±1.8	15.7±1.8	4.2±0.4	4.1±0.2	4.1±0.3	4.0±0.3	4.0±0.2
SNBC	<b>41.9±0.5</b>	42.5±0.4	42.4±0.6	42.5±0.6	42.6±0.5	4.4±0.2	4.4±0.3	4.4±0.5	4.5±0.3	4.6±0.4
wvRN	1.6±1.1	4.2±2.5	7.8±4.0	10.4±3.5	13.0±6.6	0.7±0.4	1.1±0.6	1.6±0.5	2.0±0.7	2.2±0.6
SCRN	1.7±1.3	4.2±2.1	8.3±4.1	11.8±3.1	15.0±6.2	0.7±0.4	1.1±0.5	1.7±0.5	2.1±0.5	2.4±0.5
SocDim	33.9±1.5	32.4±1.6	32.6±0.8	33.3±0.9	33.5±1.0	5.6±0.2	6.4±0.3	6.5±0.4	6.8±0.5	7.2±0.4
HeatKernel	1.3±1.0	4.3±3.3	7.7±4.3	10.5±3.8	12.8±8.7	0.6±0.4	1.0±0.7	1.5±0.6	1.7±0.6	2.0±0.7
LGC	36.7±6.5	38.9±0.1	39.0±0.1	39.0±0.1	39.1±0.1	3.0±0.3	3.0±0	3.0±0	3.0±0	2.9±0
TSVM	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
LapSVM	27.4±13.9	41.9±0.6	42.0±0.6	42.2±0.3	42.2±0.6	2.4±0.7	4.1±0.4	4.2±0.3	4.3±0.3	4.2±0.4



Thank you !