

# Stanford CS224W: Message Passing and Node Classification

CS224W: Machine Learning with Graphs  
Jure Leskovec, Stanford University  
<http://cs224w.stanford.edu>



# ANNOUNCEMENTS

- **This Thursday (10/07):** Colab 1 due, Colab 2 out
- **Next Thursday (10/14):** HW 1 due, HW 2 out
- **Office hours**
  - See <http://web.stanford.edu/class/cs224w/oh.html> for OH calendar, Zoom links, and QueueStatus link.
  - (1) Add yourself to queue, (2) Join the Zoom waiting room  
--> we will let you off the waiting room when it's your turn in the queue.

CS224W: Machine Learning with Graphs

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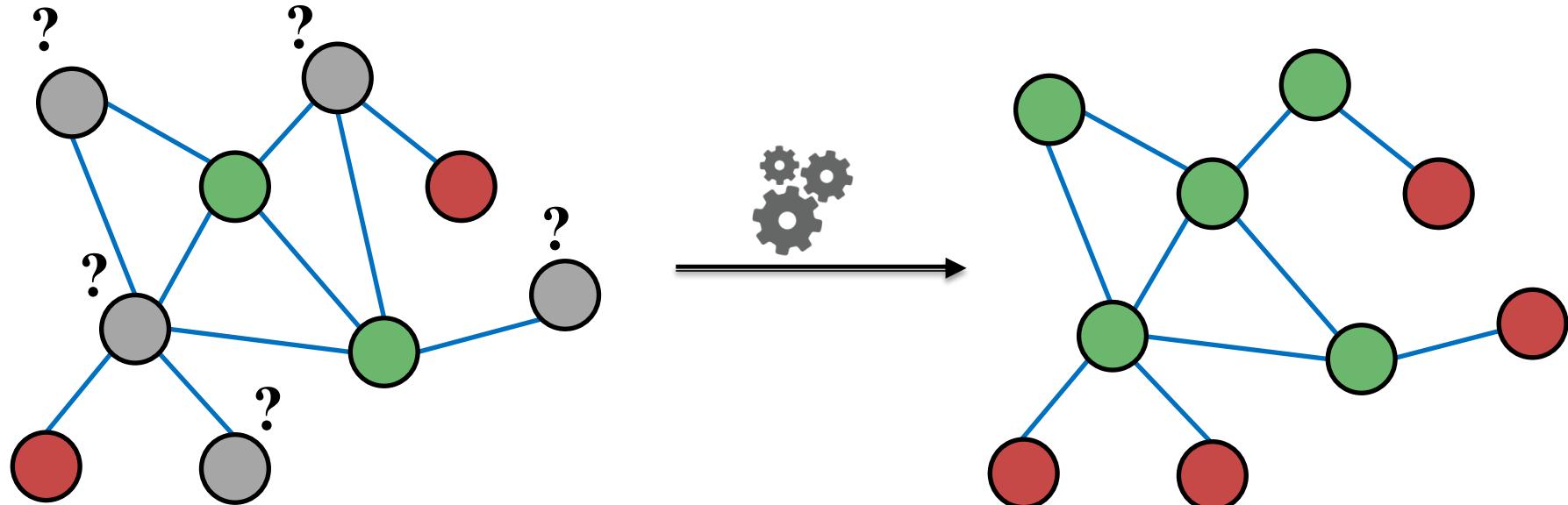
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# Today's Lecture: Outline

- **Main question today:** Given a network with labels on some nodes, how do we assign labels to all other nodes in the network?
- **Example:** In a network, some nodes are fraudsters, and some other nodes are fully trusted. **How do you find the other fraudsters and trustworthy nodes?**
- We already discussed node embeddings as a method to solve this in Lecture 3

# Example: Node Classification



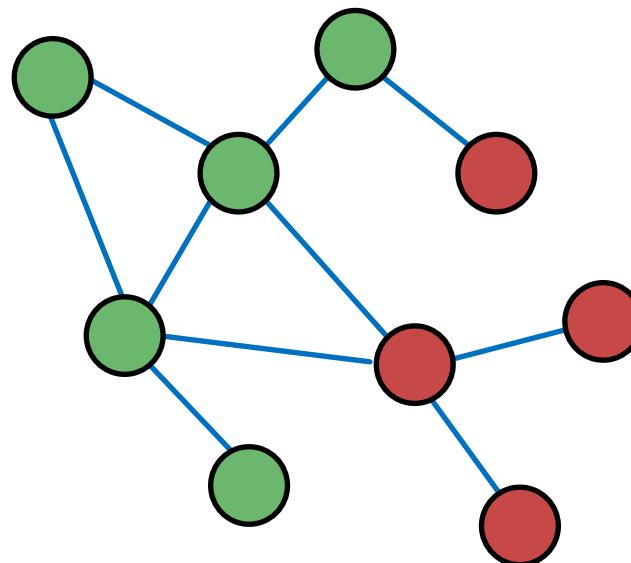
- Given labels of some nodes
- Let's predict labels of unlabeled nodes
- This is called **semi-supervised node classification**

# Today's Lecture: Outline

- **Main question today:** Given a network with labels on some nodes, how do we assign labels to all other nodes in the network?
- **Today we will discuss an alternative framework: Message passing**
- **Intuition:** **Correlations (dependencies)** exist in networks.
  - In other words: Similar nodes are connected.
  - Key concept is **collective classification**: Idea of assigning labels to all nodes in a network together.
- **We will look at three techniques today:**
  - **Relational classification**
  - **Iterative classification**
  - **Correct & Smooth**

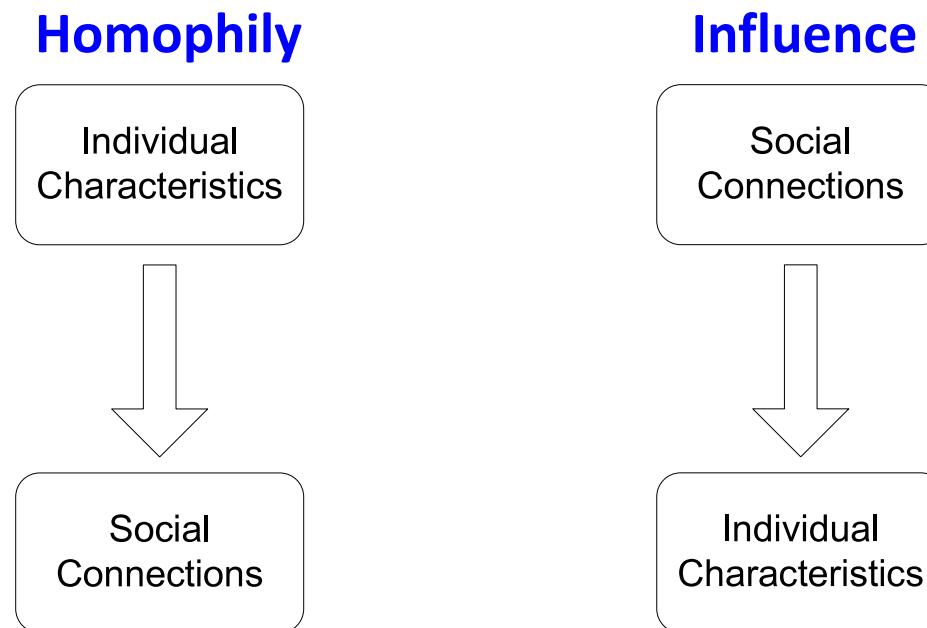
# Correlations Exist in Networks

- Behaviors of nodes are **correlated** across the links of the network
- Correlation:** Nearby nodes have the same color (belonging to the same class)



# Correlations Exist in Networks

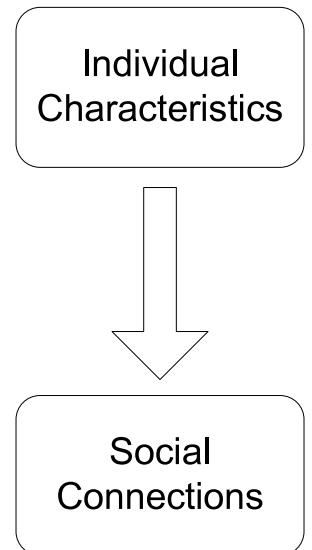
- Two explanations for why behaviors of nodes in networks are correlated:



# Social Homophily

- **Homophily:** The tendency of individuals to associate and bond with similar others
  - “*Birds of a feather flock together*”
  - It has been observed in a vast array of network studies, based on a variety of attributes (e.g., age, gender, organizational role, etc.)
  - **Example:** Researchers who focus on the same research area are **more likely to establish a connection** (meeting at conferences, interacting in academic talks, etc.)

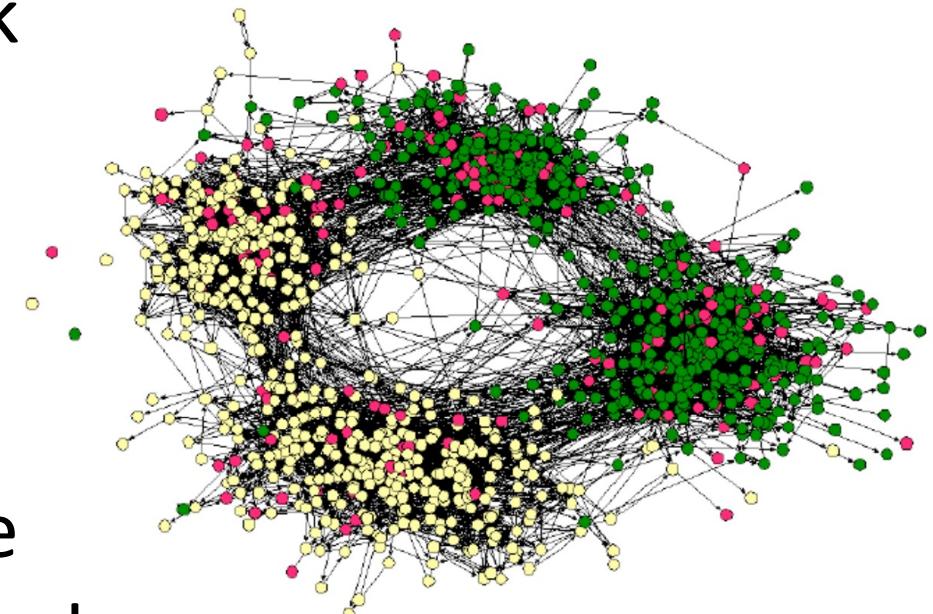
Homophily



# Homophily: Example

## Example of homophily

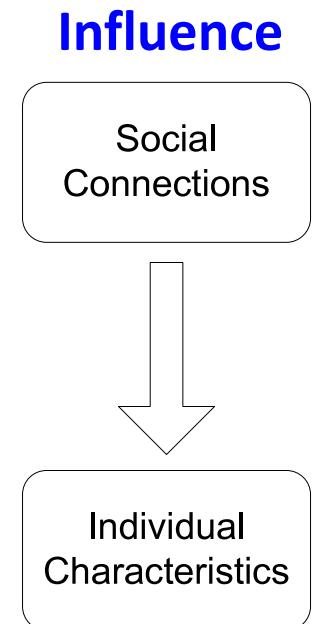
- Online social network
  - Nodes = people
  - Edges = friendship
  - Node color = interests (sports, arts, etc.)
- People with the same interest are more closely connected due to homophily



(Easley and Kleinberg, 2010)

# Social Influence: Example

- **Influence:** Social connections can influence the individual characteristics of a person.
  - **Example:** I recommend my musical preferences to my friends, until one of them grows to like my same favorite genres!



# **Stanford CS224W:**

# **How do we leverage node**

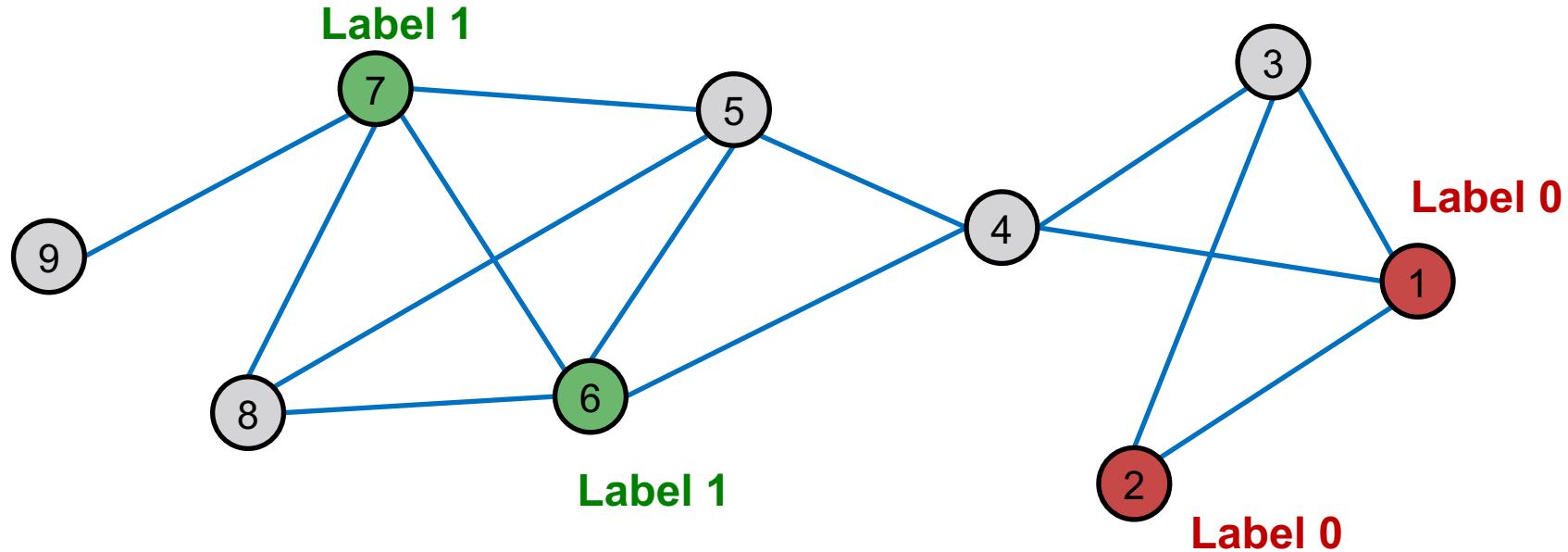
# **correlations in networks?**

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# Classification with Network Data

- How do we leverage this correlation observed in networks to help predict node labels?



How do we predict the labels for the nodes in grey?

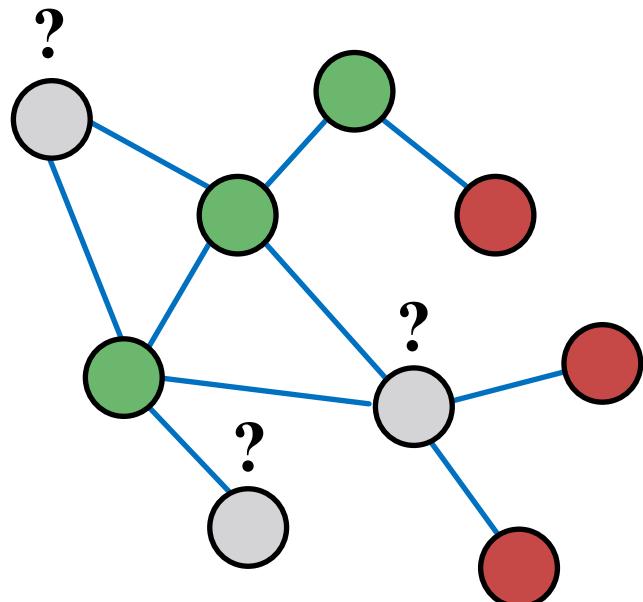
# Motivation (1)

- Similar nodes are typically close together or directly connected in the network:
  - **Guilt-by-association**: If I am connected to a node with label  $X$ , then I am likely to have label  $X$  as well.
  - **Example: Malicious/benign web page**: Malicious web pages link to one another to increase visibility, look credible, and rank higher in search engines

# Motivation (2)

- Classification label of a node  $v$  in network may depend on:
  - Features of  $v$
  - Labels of the nodes in  $v$ 's neighborhood
  - Features of the nodes in  $v$ 's neighborhood

# Semi-supervised Learning (1)



**Formal setting:**

**Given:**

- Graph
- Few labeled nodes

**Find:** Class (**red/green**) of remaining nodes

**Main assumption:** There is homophily in the network

# Semi-supervised Learning (2)

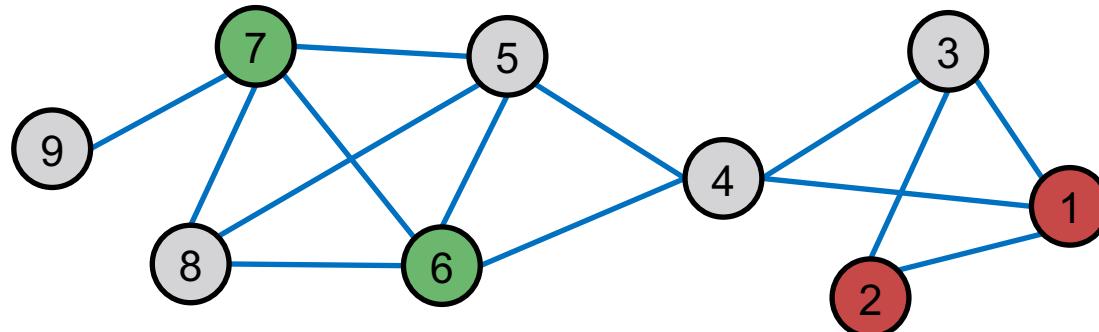
## Example task:

- Let  $A$  be a  $n \times n$  adjacency matrix over  $n$  nodes
- Let  $Y = \{0, 1\}^n$  be a vector of **labels**:
  - $Y_v = 1$  belongs to **Class 1**
  - $Y_v = 0$  belongs to **Class 0**
  - There are **unlabeled** node needs to be classified
- **Goal:** Predict which **unlabeled** nodes are likely **Class 1**, and which are likely **Class 0**

# Problem Setting

- How to predict the labels  $Y_v$  for the unlabeled nodes  $v$  (in grey color)?
- Each node  $v$  has a feature vector  $f_v$
- Labels for some nodes are given (1 for green, 0 for red)
- Task: Find  $P(Y_v)$  given all features and the network

$$P(Y_v) = ?$$



# Example applications:

- **Many applications under this setting:**
  - Document classification
  - Part of speech tagging
  - Link prediction
  - Optical character recognition
  - Image/3D data segmentation
  - Entity resolution in sensor networks
  - Spam and fraud detection

# Overview of What is Coming

- We focus on semi-supervised binary node classification
  - We will introduce three approaches:
    - Relational classification
    - Iterative classification
    - Correct & Smooth
- local classifier:* Used for initial label assignment  
network info used
- apply it in rounds*
- Collective Classification:* Markov Assumption (only depends on neighbors)  
degree 1.

# **Stanford CS224W:** **Relational Classification**

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# Probabilistic Relational Classifier (1)

- **Idea:** Propagate node labels across the network
  - Class probability  $Y_v$  of node  $v$  is a weighted average of class probabilities of its neighbors.
- For **labeled nodes**  $v$ , initialize label  $Y_v$  with ground-truth label  $Y_v^*$ .
- For **unlabeled nodes**, initialize  $Y_v = 0.5$ .
- **Update** all nodes in a random order until convergence or until maximum number of iterations is reached.

# Probabilistic Relational Classifier (2)

- **Update** for each node  $v$  and label  $c$  (e.g. 0 or 1)

$$P(Y_v = c) = \frac{1}{\sum_{(v,u) \in E} A_{v,u}} \sum_{(v,u) \in E} A_{v,u} P(Y_u = c)$$

*average likelihood of neighbors*

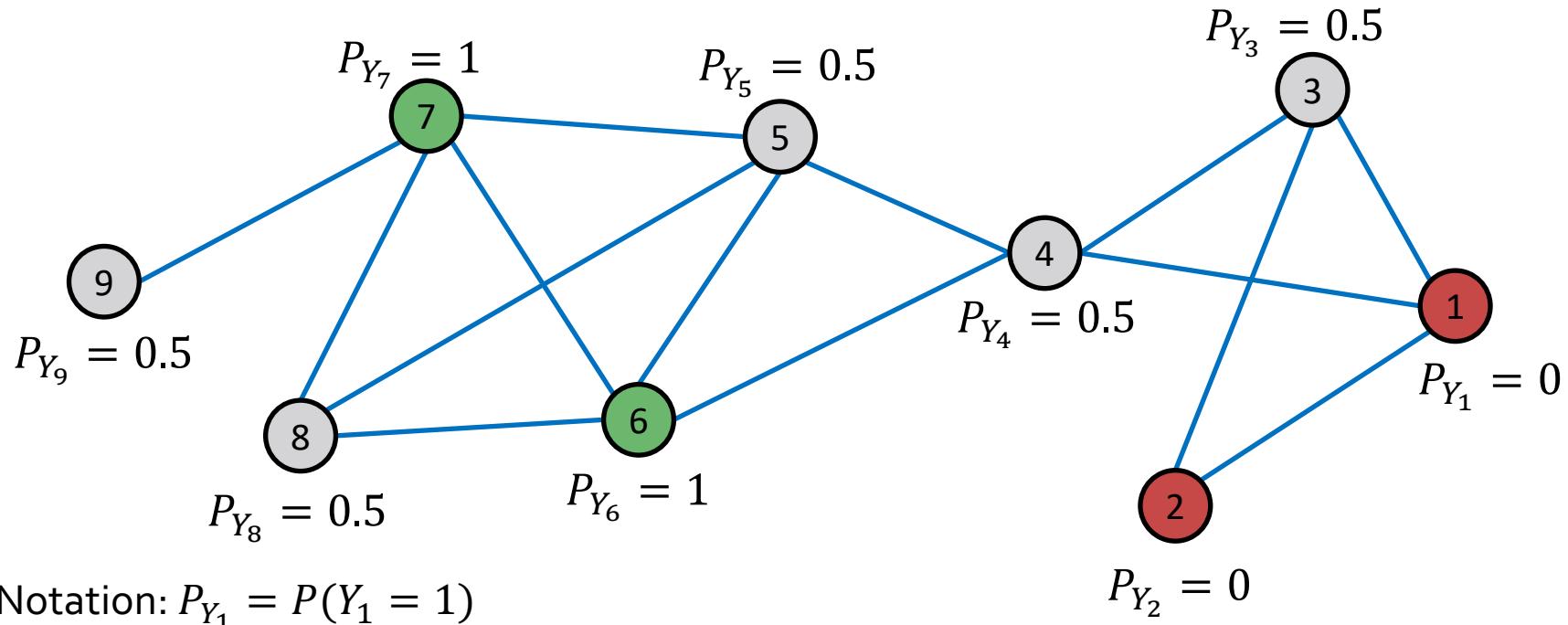
*Sum of weights of edges & adjacent with  $v$ .*

- If edges have strength/weight information,  $A_{v,u}$  can be the edge weight between  $v$  and  $u$
- $P(Y_v = c)$  is the probability of node  $v$  having label  $c$
- **Challenges:**
  - Convergence is not guaranteed
  - Model cannot use node feature information

# Example: Initialization

## Initialization:

- All labeled nodes with their labels
- All unlabeled nodes 0.5 (belonging to class 1 with probability 0.5)

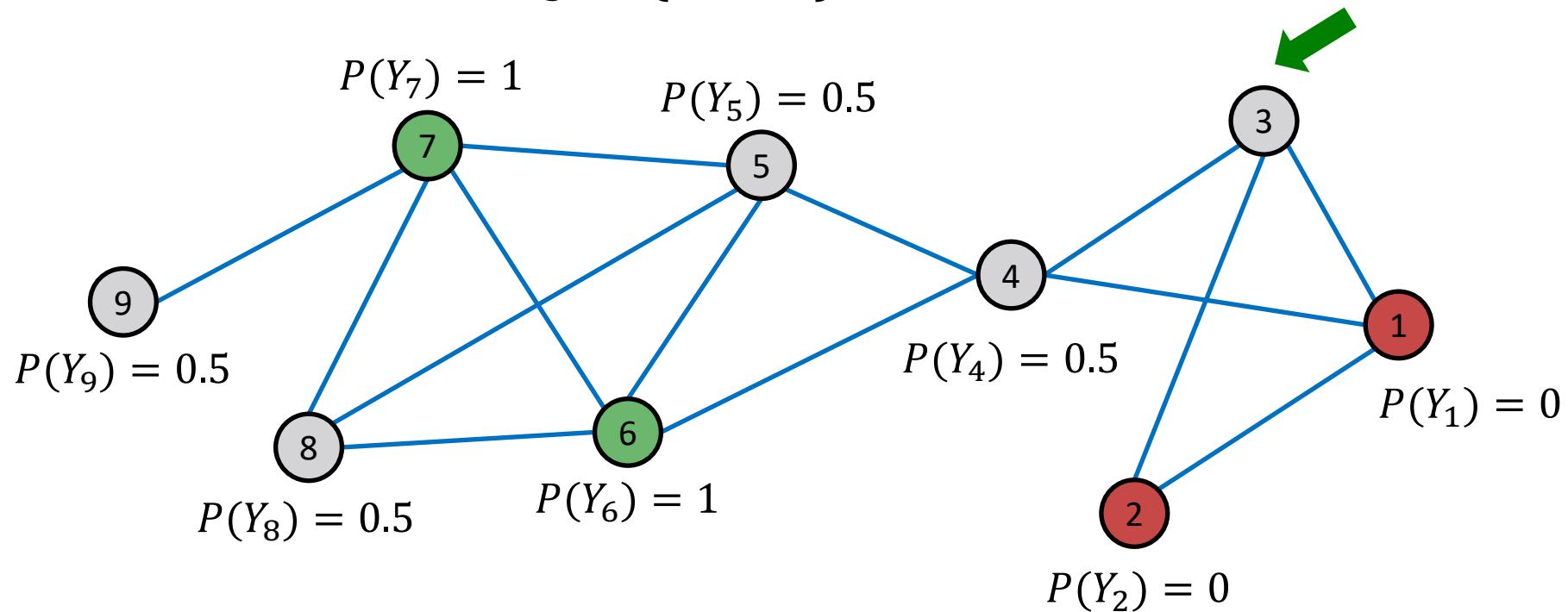


# Example: 1<sup>st</sup> Iteration, Update Node 3

- Update for the 1<sup>st</sup> Iteration:

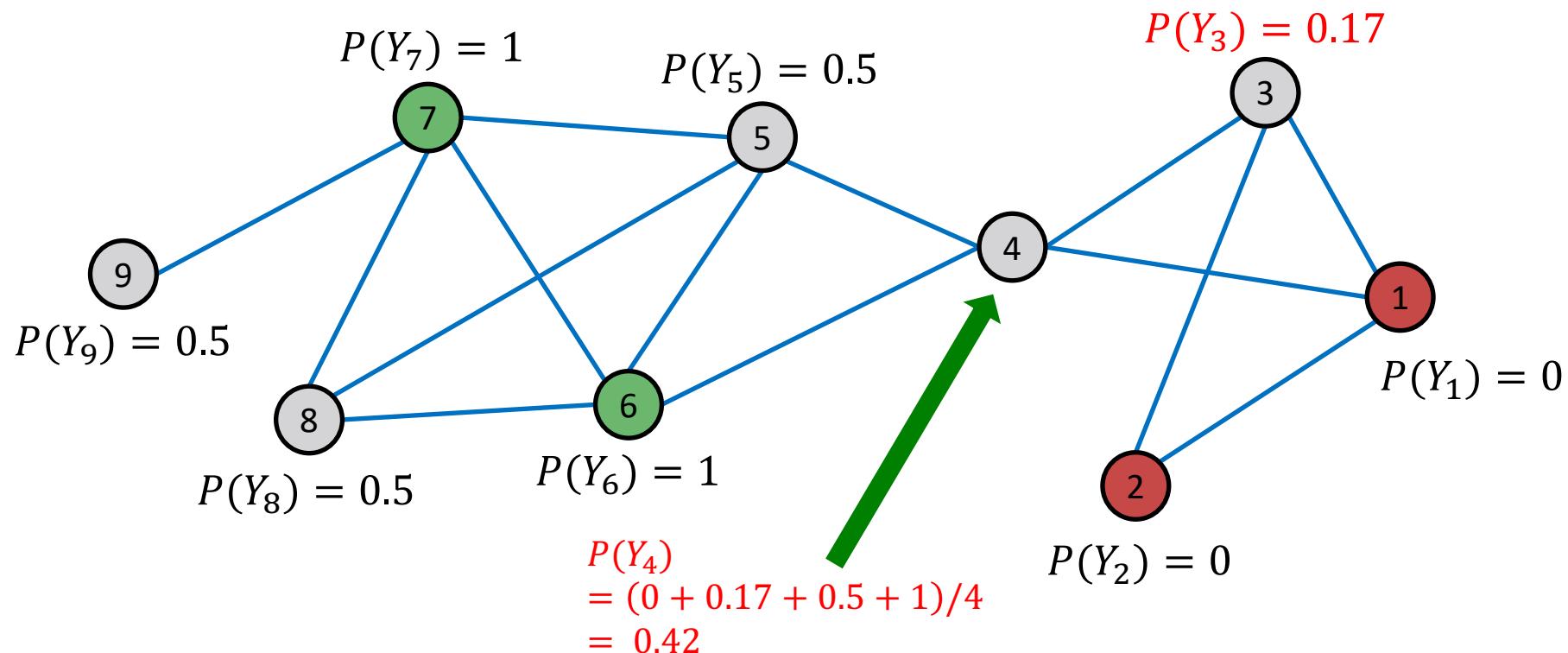
- For node 3,  $N_3 = \{1, 2, 4\}$

$$P(Y_3) = (0 + 0 + 0.5)/3 = 0.17$$



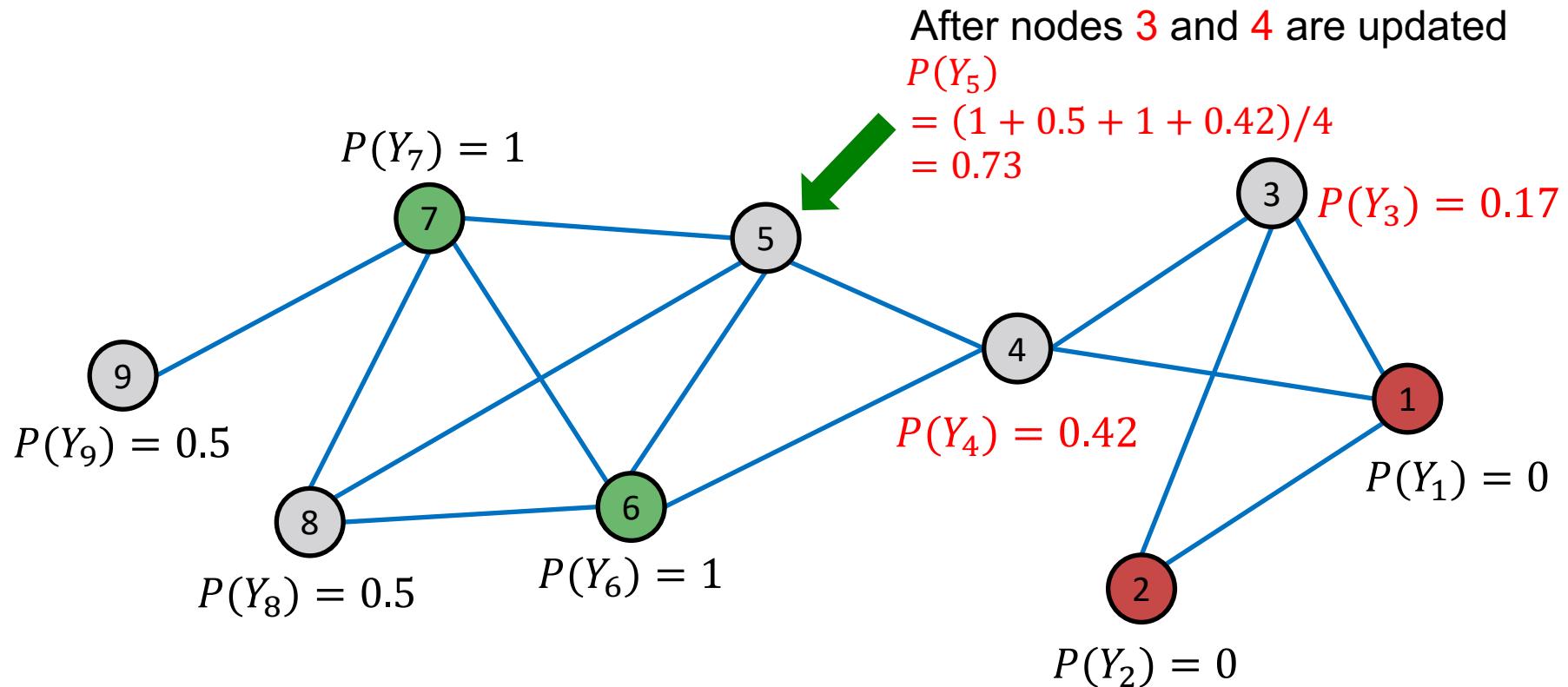
# Example: 1<sup>st</sup> Iteration, Update Node 4

- Update for the 1<sup>st</sup> Iteration:
  - For node 4,  $N_4 = \{1, 3, 5, 6\}$



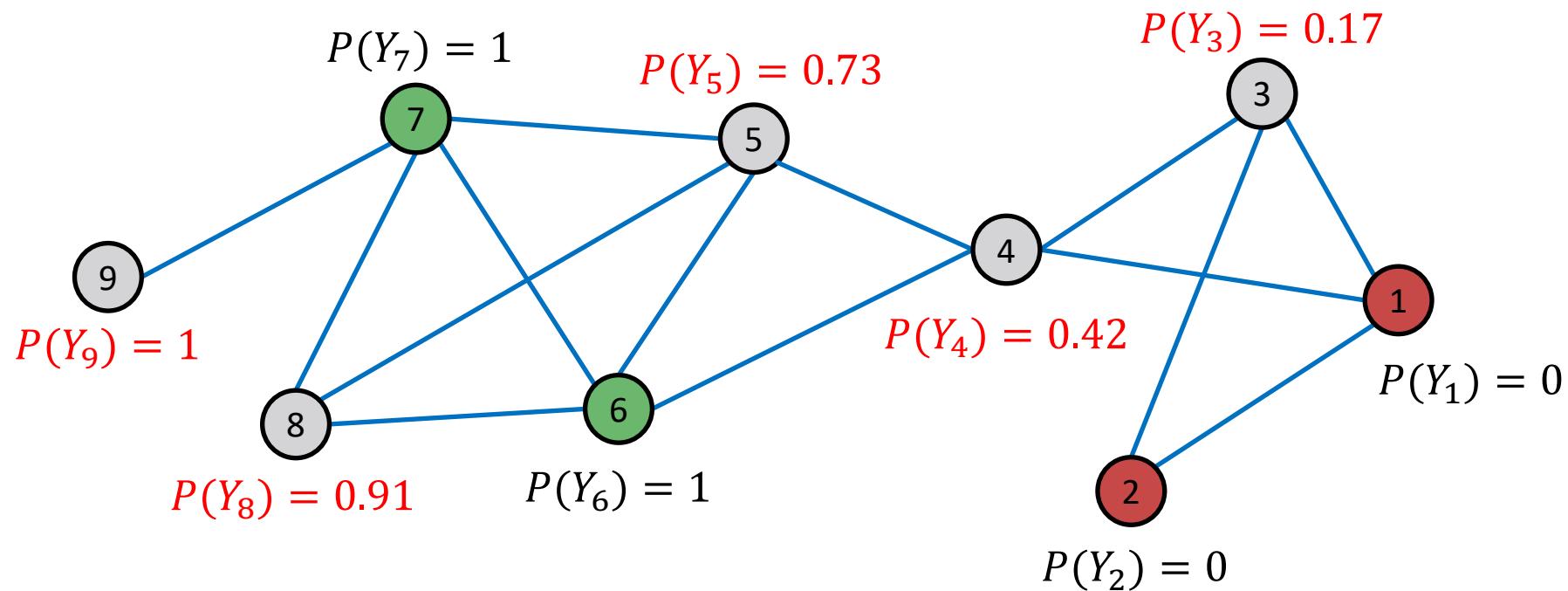
# Example: 1<sup>st</sup> Iteration, Update Node 5

- Update for the 1<sup>st</sup> Iteration:
  - For node 5,  $N_5 = \{4, 6, 7, 8\}$



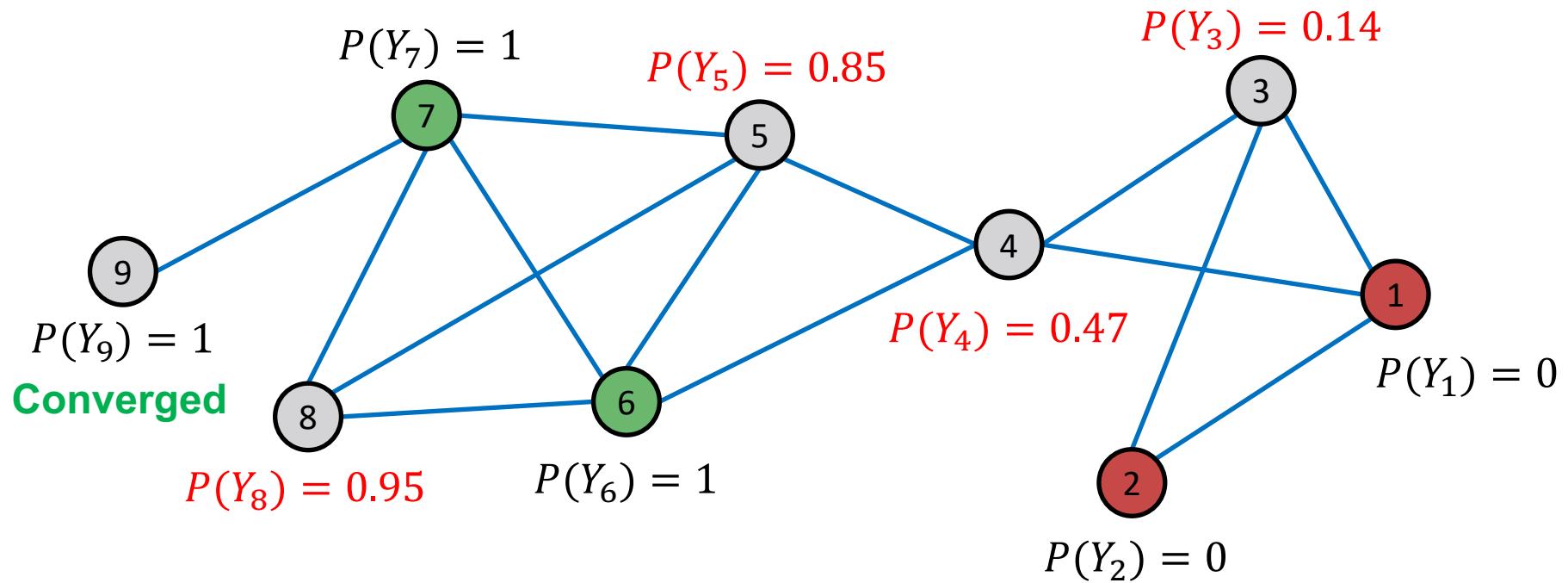
# Example: After 1<sup>st</sup> Iteration

After Iteration 1 (a round of updates for all unlabeled nodes)



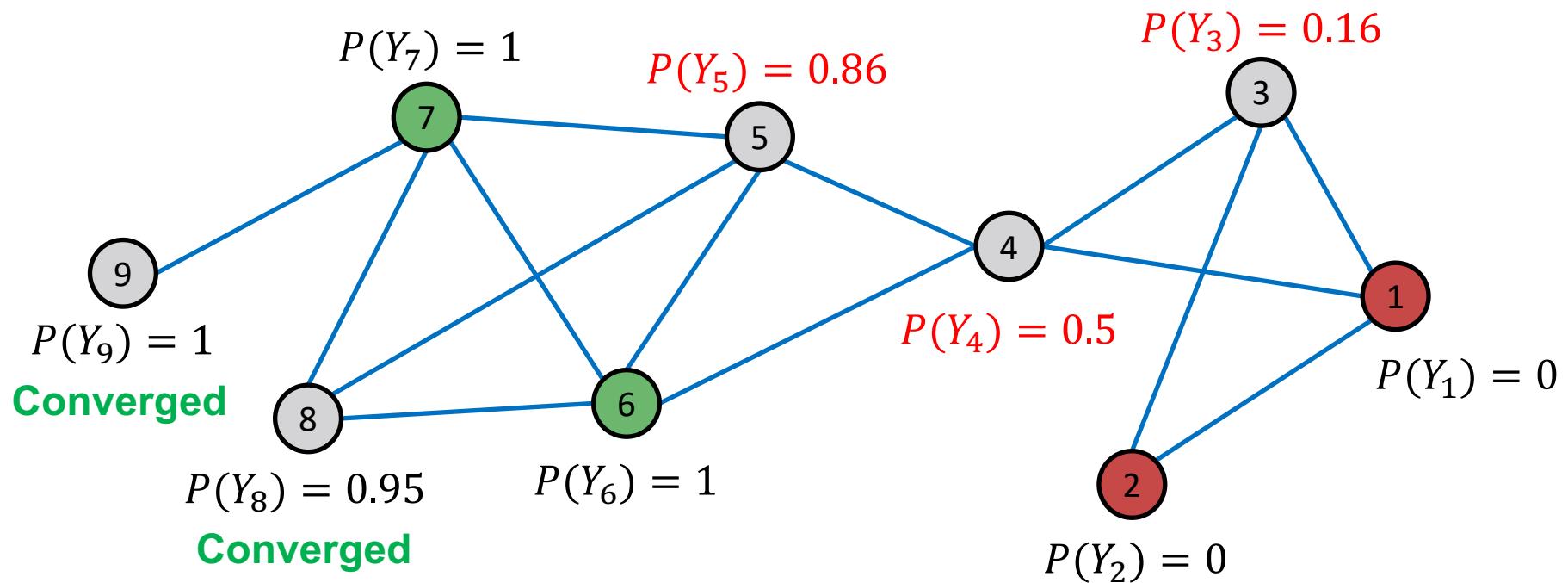
# Example: After 2<sup>nd</sup> Iteration

After Iteration 2



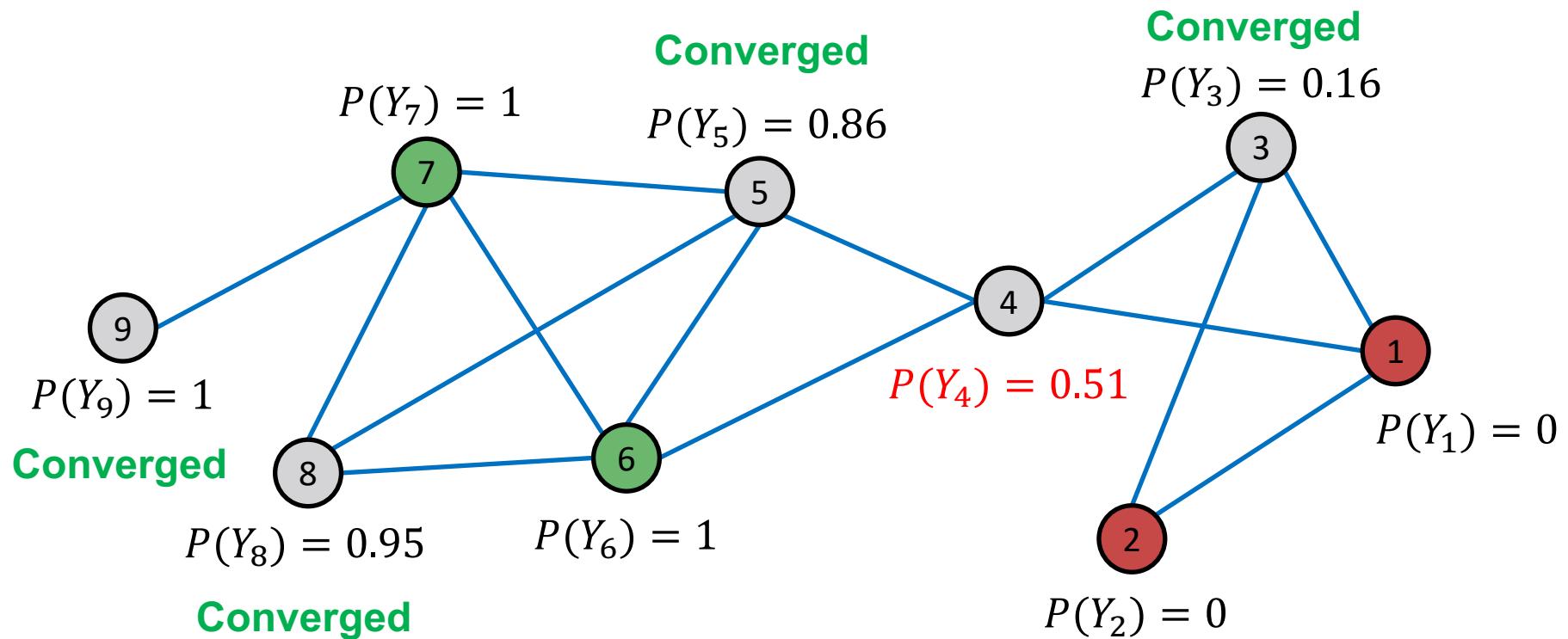
# Example: After 3<sup>rd</sup> Iteration

After Iteration 3



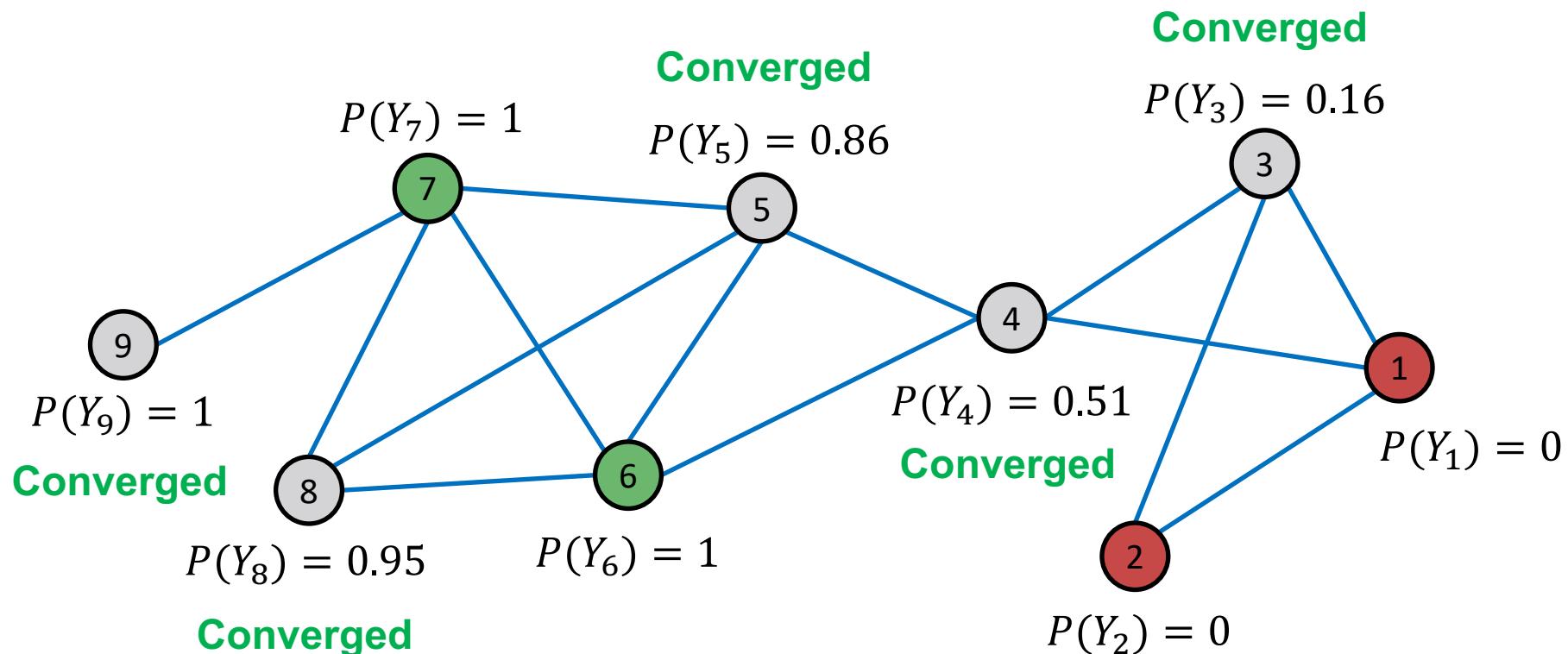
# Example: After 4<sup>th</sup> Iteration

After Iteration 4



# Example: Convergence

- All scores stabilize after 4 iterations. We therefore predict:
  - Nodes 4, 5, 8, 9 belong to class 1 ( $P_{Y_v} > 0.5$ )
  - Nodes 3 belongs to class 0 ( $P_{Y_v} < 0.5$ )



# Stanford CS224W: Iterative Classification

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# Iterative Classification

- Relational classifier **does not use node attributes.**
- How can one leverage them?
- **Main idea of iterative classification:** Classify node  $v$  based on its **attributes**  $f_v$ , as well as **labels**  $\mathbf{z}_v$  of neighbor set  $N_v$ .

# Iterative Classification

- **Input: Graph**

- $f_v$  : feature vector for node  $v$
- Some nodes  $v$  are labeled with  $Y_v$

- **Task:** Predict label of unlabeled nodes

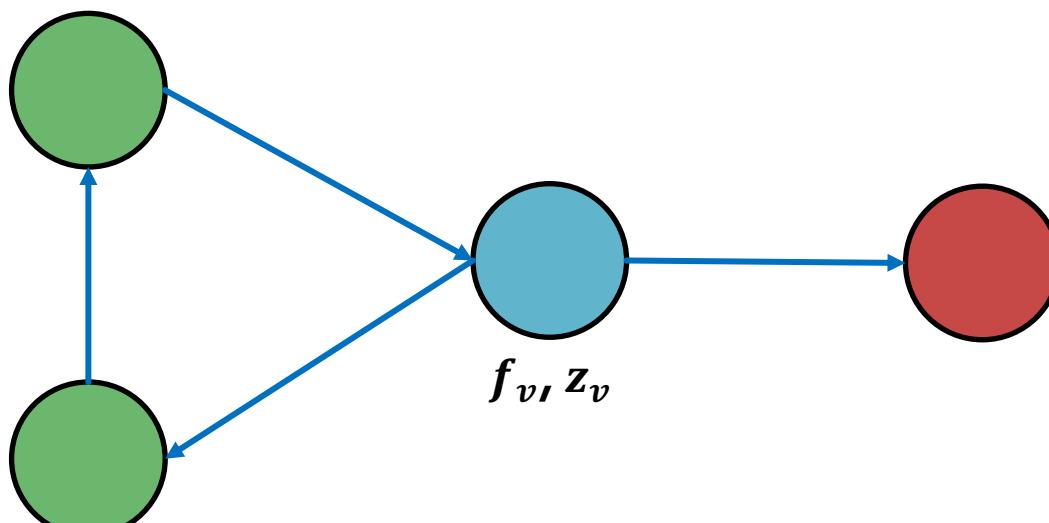
- **Approach: Train two classifiers:**

- $\phi_1(f_v)$  = Predict node label based on node feature vector  $f_v$ . This is called **base classifier**.
- $\phi_2(f_v, z_v)$  = Predict label based on node feature vector  $f_v$  and summary  $z_v$  of labels of  $v$ 's neighbors. This is called **relational classifier**.

# Computing the Summary $z_v$

How do we compute the summary  $z_v$  of labels of  $v$ 's neighbors  $N_v$ ?

- $z_v$  = vector that captures labels around node  $v$ 
  - Histogram of the number (or fraction) of each label in  $N_v$
  - Most common label in  $N_v$
  - Number of different labels in  $N_v$



# Architecture of Iterative Classifiers

- **Phase 1: Classify based on node attributes alone**
  - On the labeled **training set**, train two classifiers:
    - **Base classifier:**  $\phi_1(f_v)$  to predict  $Y_v$  based on  $f_v$
    - **Relational classifier:**  $\phi_2(f_v, z_v)$  to predict  $Y_v$  based on  $f_v$  and summary  $z_v$  of labels of  $v$ 's neighbors
- **Phase 2: Iterate till convergence**
  - On **test set**, set labels  $Y_v$  based on the classifier  $\phi_1$ , compute  $z_v$  and **predict the labels with  $\phi_2$**
  - **Repeat** for each node  $v$ :
    - Update  $z_v$  based on  $Y_u$  for all  $u \in N_v$
    - Update  $Y_v$  based on the new  $z_v$  ( $\phi_2$ )
  - Iterate until class labels stabilize or max number of iterations is reached
  - **Note:** Convergence is not guaranteed

$\phi_1$ ,  
Design  
initial  
labels.

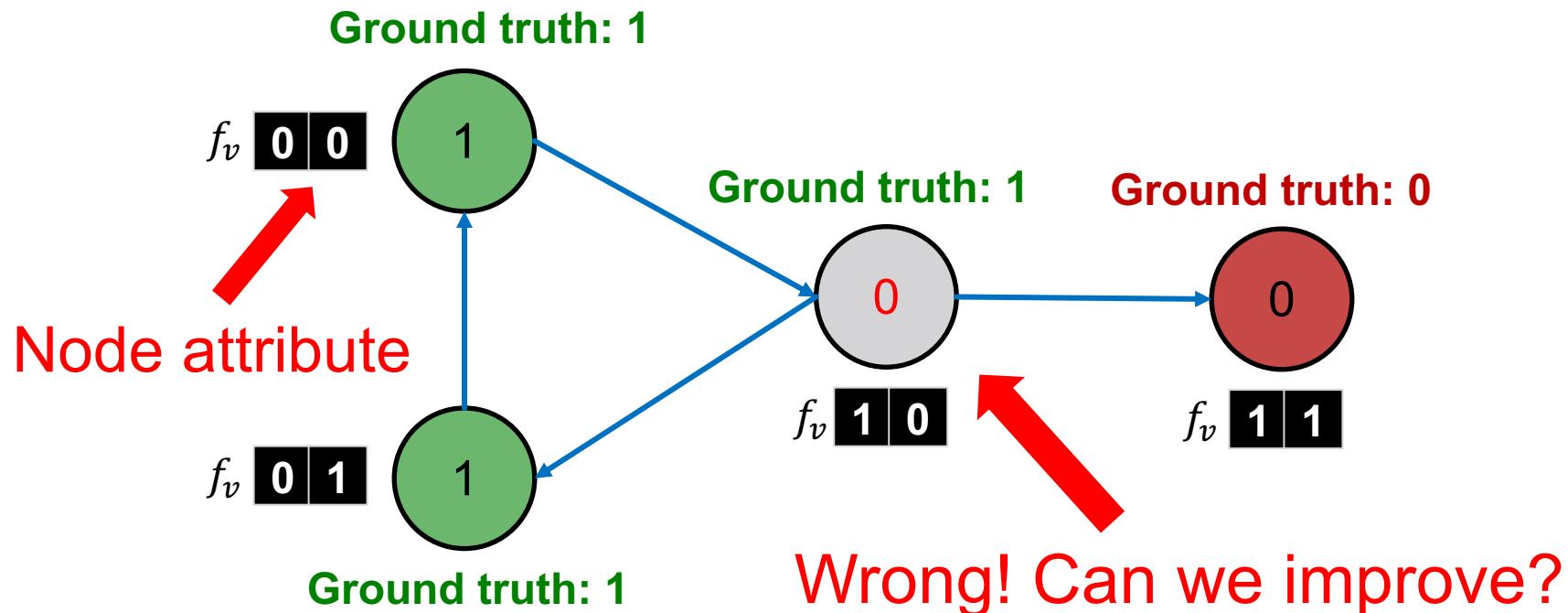
# Example: Web Page Classification (1)

- **Input:** Graph of web pages
- **Node:** Web page
- **Edge:** Hyper-link between web pages
  - **Directed edge:** a page points to another page
- **Node features:** Webpage description
  - For simplicity, we only consider two binary features
- **Task:** Predict the topic of the webpage

① Used words to predict the topic / ② rely on links too.

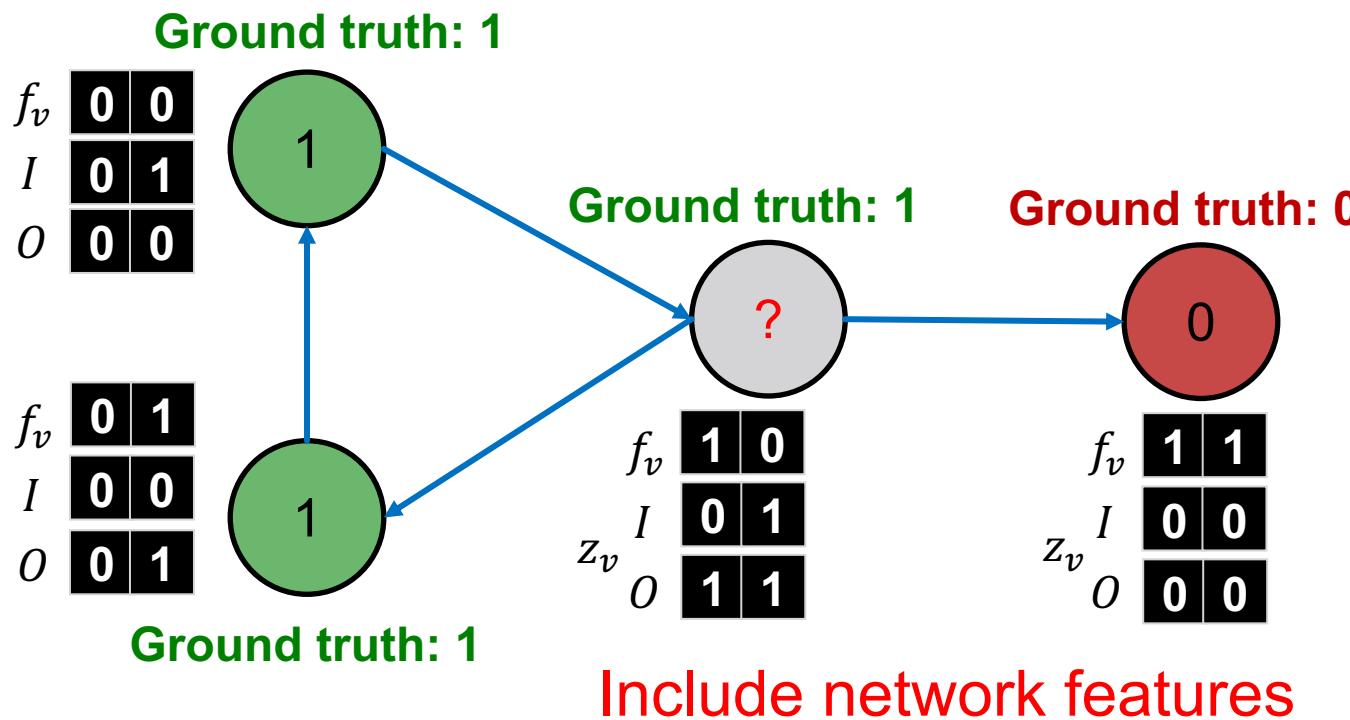
# Example: Web Page Classification (2)

- **Baseline:** Train a classifier (e.g., linear classifier) to classify pages based on node attributes.



# Example: Web Page Classification (3)

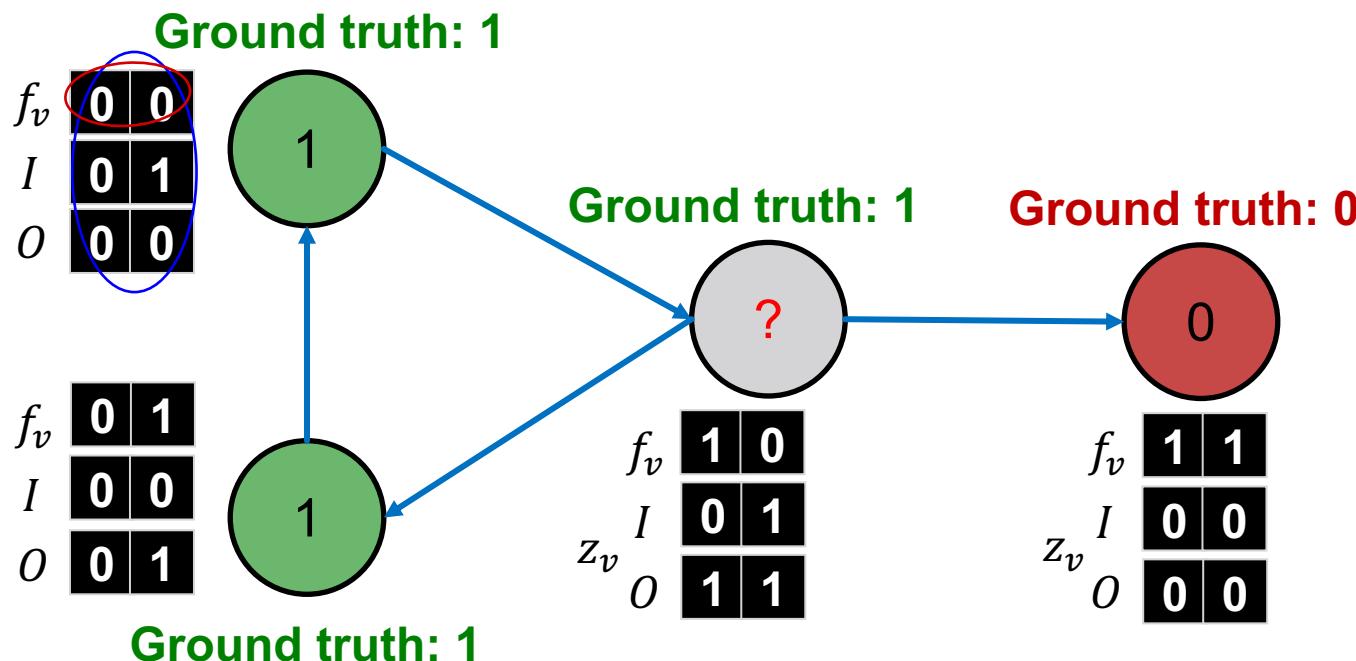
- Each node maintains **vectors**  $\mathbf{z}_v$  of neighborhood labels:
  - $I$  = **Incoming** neighbor label information vector.
  - $O$  = **Outgoing** neighbor label information vector.
    - $I_0 = 1$  if at least one of the incoming pages is labelled 0.
    - Similar definitions for  $I_1, O_0$ , and  $O_1$



# Iterative Classifier – Step 1

- On training labels, train two classifiers:
  - Node attribute vector only:  $\phi_1(f_v)$
  - Node attribute and link vectors  $z_v$ :  $\phi_2(f_v, z_v)$

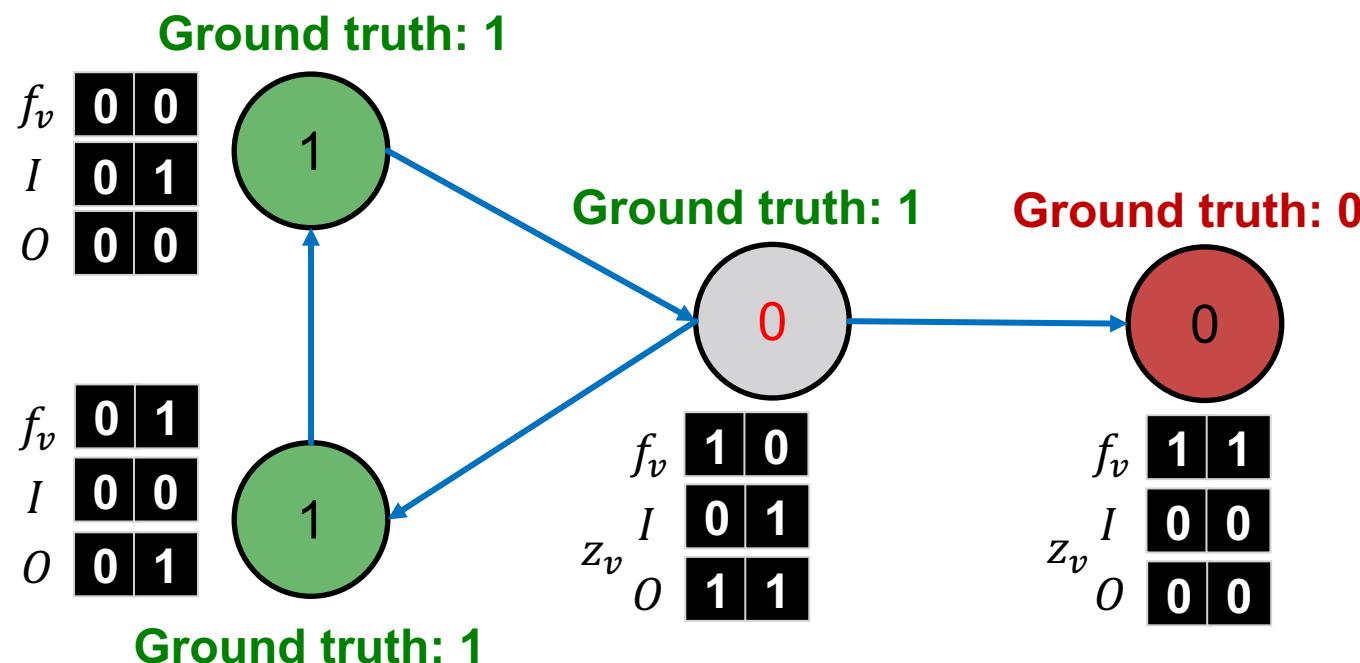
1. Train classifiers
2. Apply classifier to unlab. set
3. Iterate
  - 4. Update relational features  $z_v$
  - 5. Update label  $Y_v$



# Iterative Classifier – Step 2

- On the **unlabeled set**:
  - Use trained node feature vector classifier  $\phi_1$  to set  $Y_v$

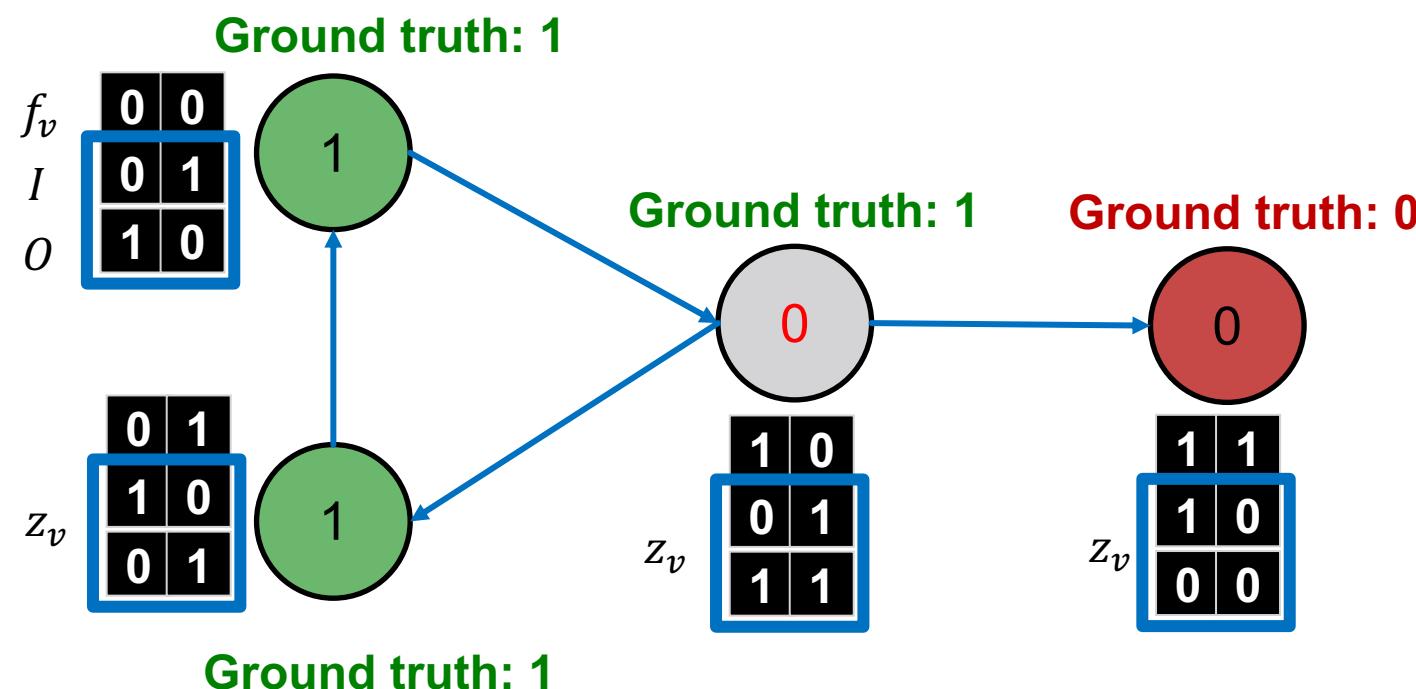
- Train classifiers
- Apply classifier to unlab. set**
- Iterate
  - Update relational features  $z_v$
  - Update label  $Y_v$



# Iterative Classifier – Step 3.1

- Update  $z_v$  for all nodes:

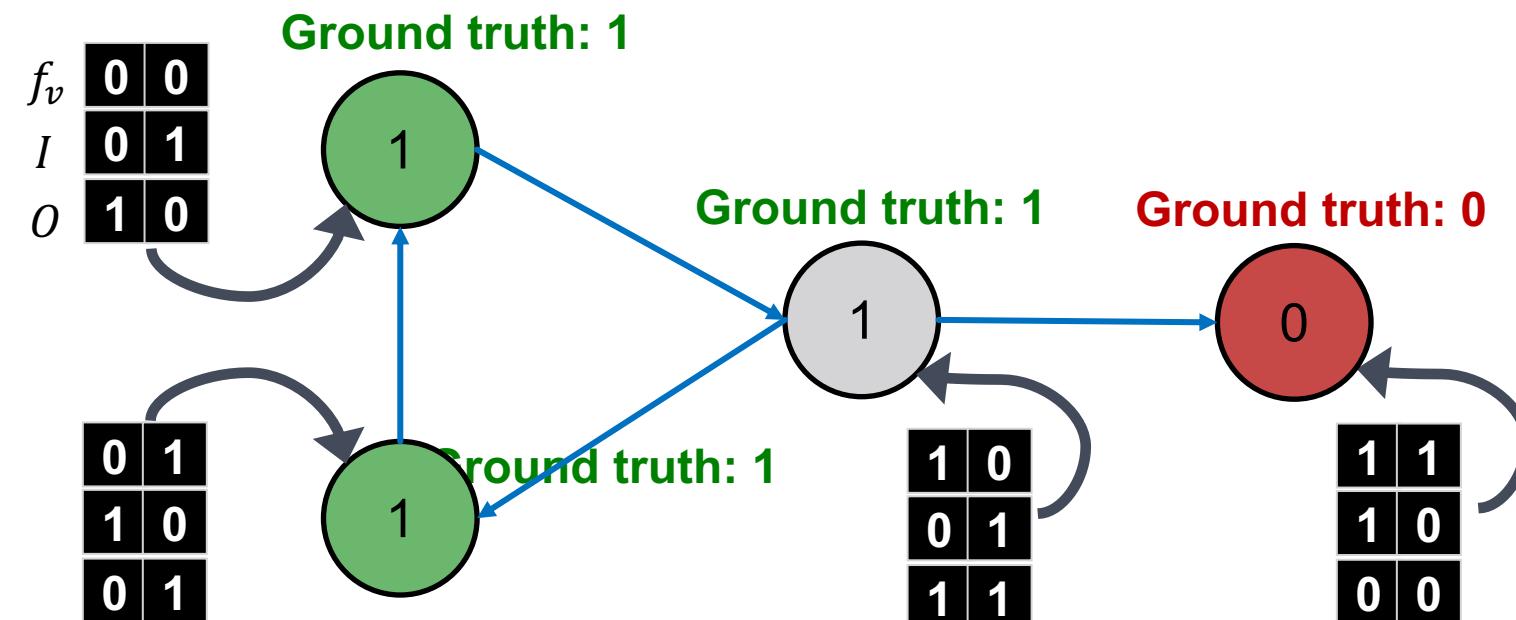
1. Train classifiers
2. Apply classifier to unlab. set
3. Iterate
4. Update relational features  $z_v$
5. Update label  $Y_v$



# Iterative Classifier – Step 3.2

- Re-classify all nodes with  $\phi_2$ :

1. Train classifiers
2. Apply classifier to unlab. set
3. Iterate
4. Update relational features  $z_v$
5. Update label  $Y_v$



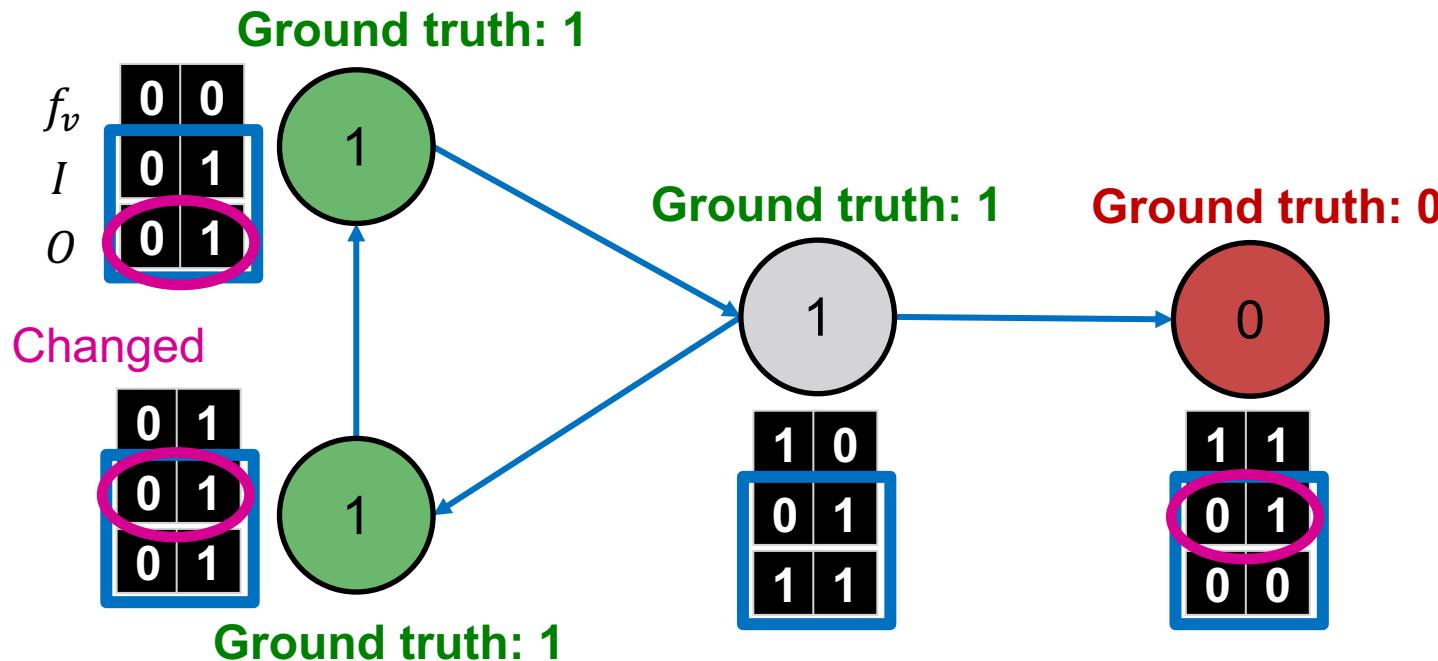
Now it's correct prediction!

# Iterative Classifier – Iterate

## ■ Continue until convergence

- Update  $z_v$  based on  $Y_v$
- Update  $Y_v = \phi_2(f_v, z_v)$

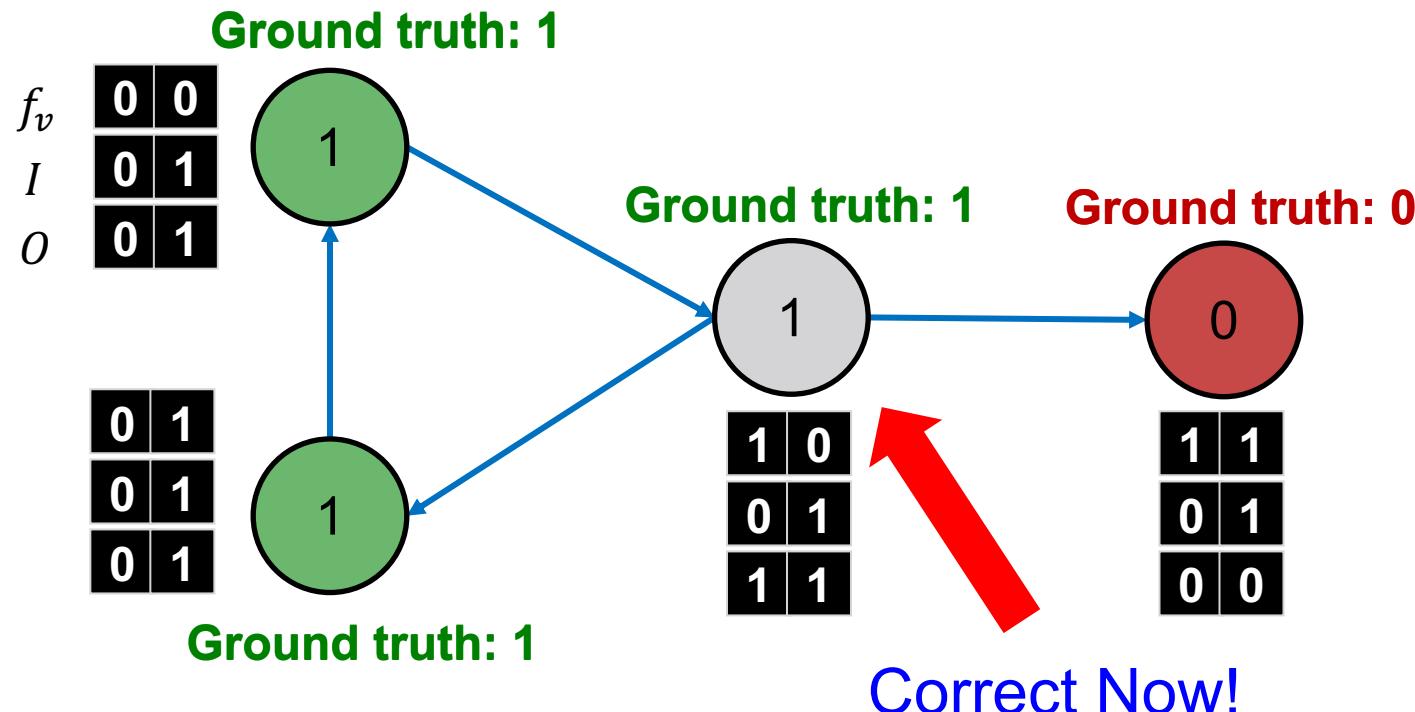
1. Train classifiers
2. Apply classifier to unlab. set
- 3. Iterate**
4. Update relational features  $z_v$
5. Update label  $Y_v$



# Iterative Classifier – Final Prediction

## ■ Stop iteration

- After convergence or when maximum iterations are reached



# Summary

- We talked about 2 approaches to collective classification
- Relational classification
  - Iteratively update probabilities of node belonging to a label class based on its neighbors
- Iterative classification
  - Improve over collective classification to handle attribute/feature information
  - Classify node  $v$  based on its **features** as well as **labels** of neighbors

# **Stanford CS224W:** **Collective Classification:** **Correct & Smooth**

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# Correct & Smooth = Message Passing

- Last, we introduce **C&S**, recent state-of-the-art collective classification method.

## Leaderboard for ogbn-products

The classification accuracy on the test and validation sets. The higher, the better.

Package:  $\geq 1.1.1$

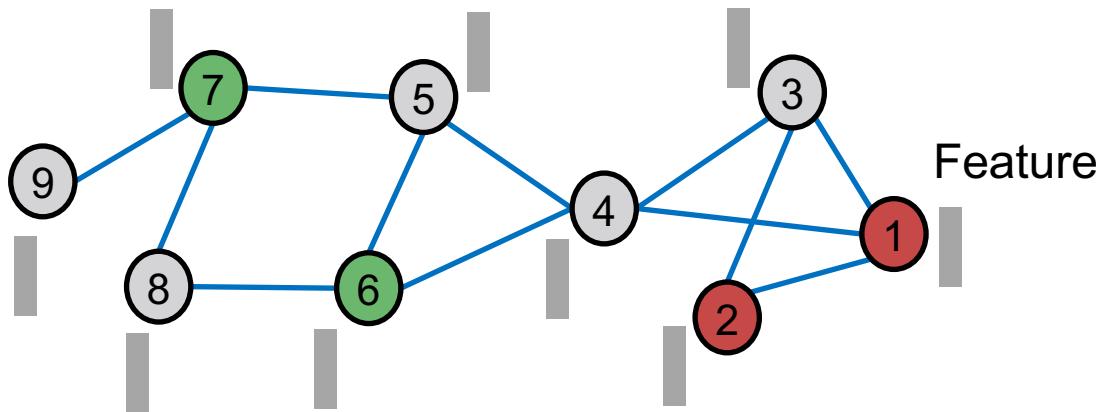
Rank	Method	Test Accuracy	Validation Accuracy	Contact	References	#Params	Hardware	Date
1	SAGN+SLE (4 stages)+C&S	0.8485 ± 0.0010	0.9302 ± 0.0003	Chuxiong Sun (CTRI)	Paper, Code	2,179,678	Tesla V100 (16GB GPU)	Sep 21, 2021
2	SAGN+SLE (4 stages)	0.8468 ± 0.0012	0.9309 ± 0.0007	Chuxiong Sun (CTRI)	Paper, Code	2,179,678	Tesla V100 (16GB GPU)	Sep 21, 2021
3	GAMLP+RLU	0.8459 ± 0.0010	0.9324 ± 0.0005	Wentao Zhang (PKU Tencent Joint Lab)	Paper, Code	3,335,831	Tesla V100 (32GB)	Aug 19, 2021
4	Spec-MLP-Wide + C&S	0.8451 ± 0.0006	0.9132 ± 0.0010	Huixuan Chi (AML@ByteDance)	Paper, Code	406,063	Tesla V100 (32GB)	Jul 27, 2021
5	SAGN+SLE	0.8428 ± 0.0014	0.9287 ± 0.0003	Chuxiong Sun	Paper, Code	2,179,678	Tesla V100 (16GB GPU)	Apr 19, 2021
6	MLP + C&S	0.8418 ± 0.0007	0.9147 ± 0.0009	Horace He (Cornell)	Paper, Code	96,247	GeForce RTX 2080 (11GB GPU)	Oct 27, 2020

**C&S** tops the current OGB leaderboard!

[OGB leaderboard](#) snapshot at Oct 1<sup>st</sup>, 2021

# Correct & Smooth

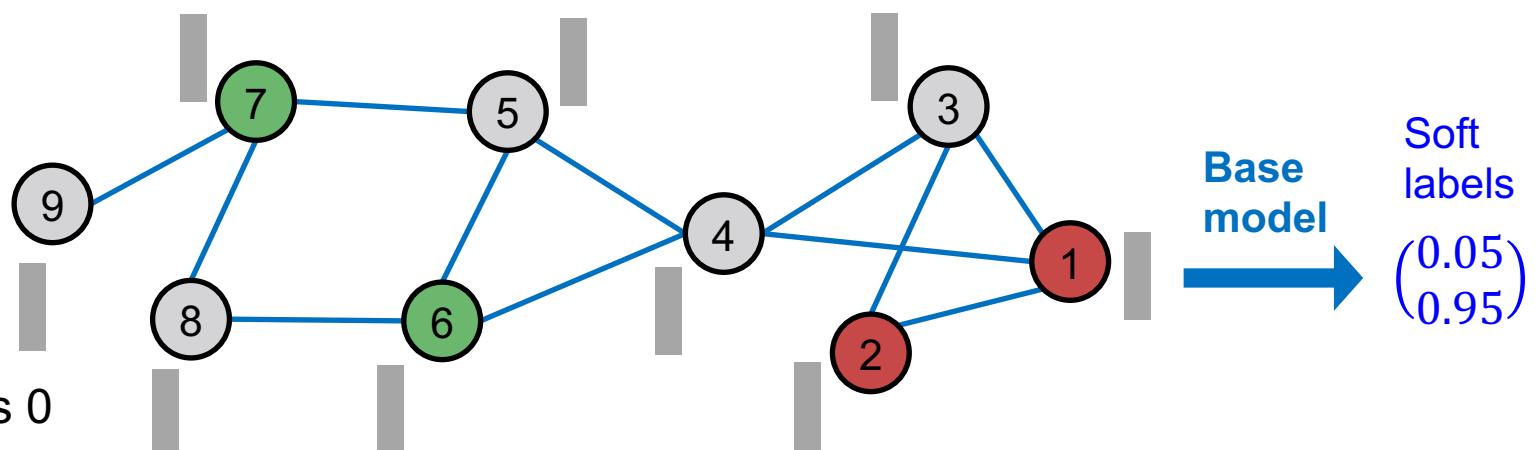
- **Setting:** A partially labeled graph and features over nodes.



- **C&S follows the three-step procedure:**
  1. Train base predictor
  2. Use the base predictor to predict soft labels of all nodes.
  3. **Post-process the predictions using graph structure** to obtain the final predictions of all nodes.

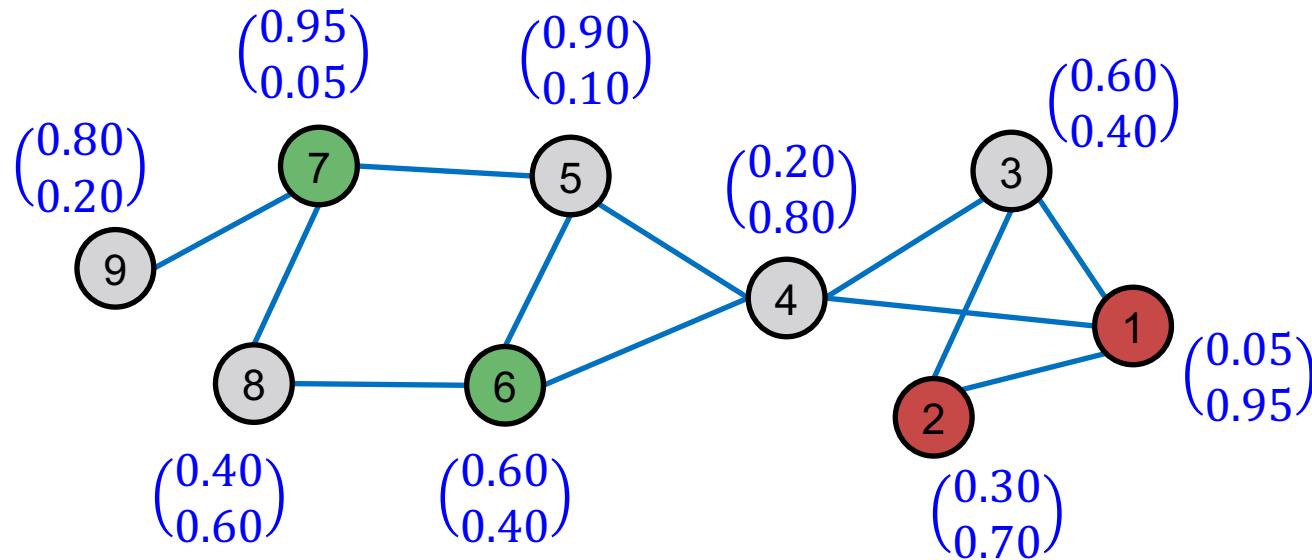
# C&S: (1) Train Base Predictor

- (1) Train a **base predictor** that predict **soft labels** (class probabilities) over all nodes.
  - Labeled nodes are used for train/validation data.
  - **Base predictor** can be simple:
    - Linear model/Multi-Layer-Perceptron(MLP) over node features



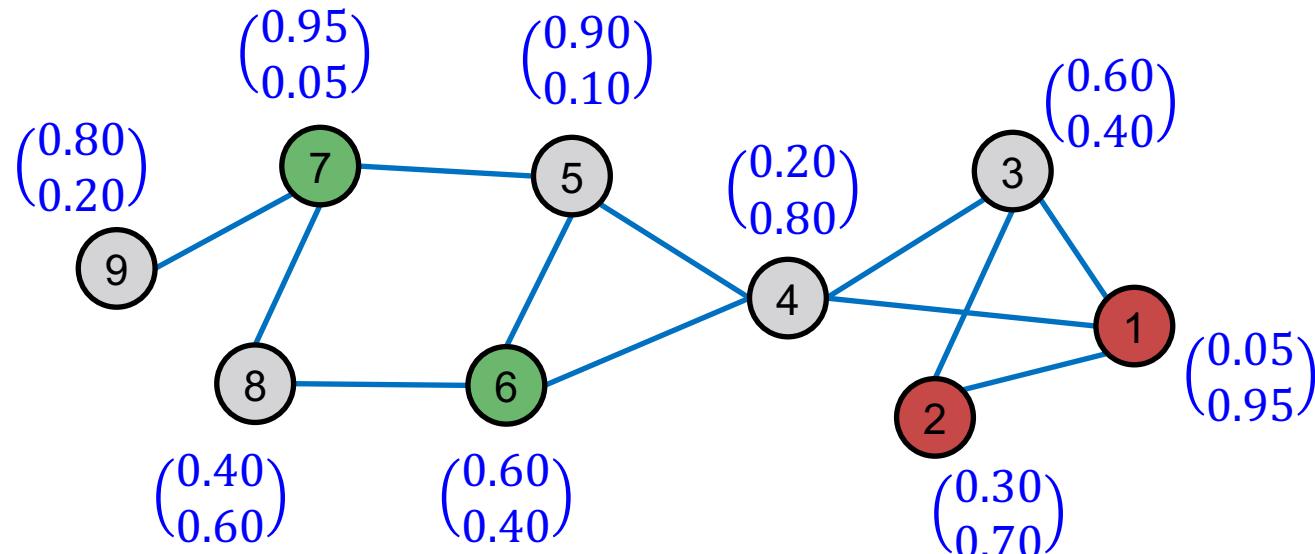
# C&S: (2) Predict Over All Nodes

- (2) Given a trained **base predictor**, we apply it to obtain **soft labels** for all the nodes.
  - We expect these soft labels to be decently accurate.
  - **Can we use graph structure to post-process the predictions to make them more accurate?**



# C&S: (3) Post-Process Predictions

- (3) C&S uses the 2-step procedure to post-process the **soft predictions**.
  1. Correct step
  2. Smooth step



# C&S Post-Processing: Correct Step

- The key idea is that we expect errors in the base prediction to be positively correlated along edges in the graph.
  - In other words, an error at node  $u$  increases the chance of a similar error at neighbors of  $u$ .
  - Thus, we should “spread” such uncertainty over the graph.

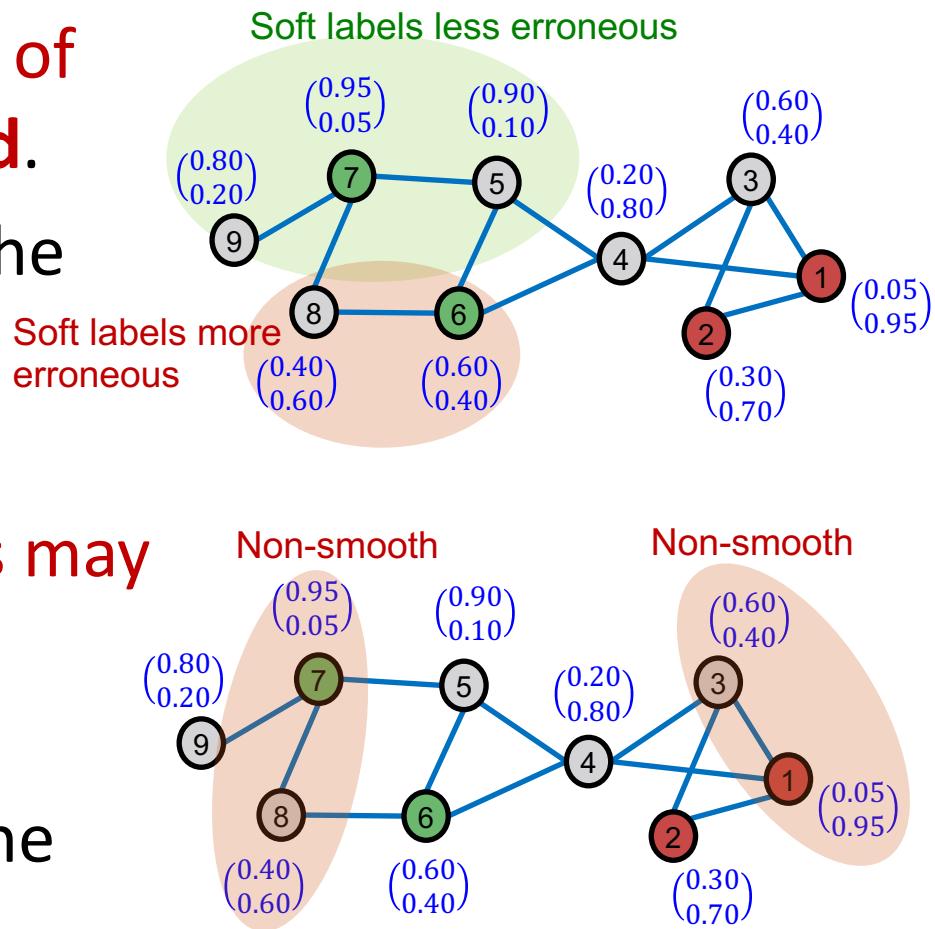
# Intuition of Correct & Smooth

## ■ Correct step

- The degree of the errors of the soft labels are **biased**.
- We need to correct for the error bias.

## ■ Smooth step

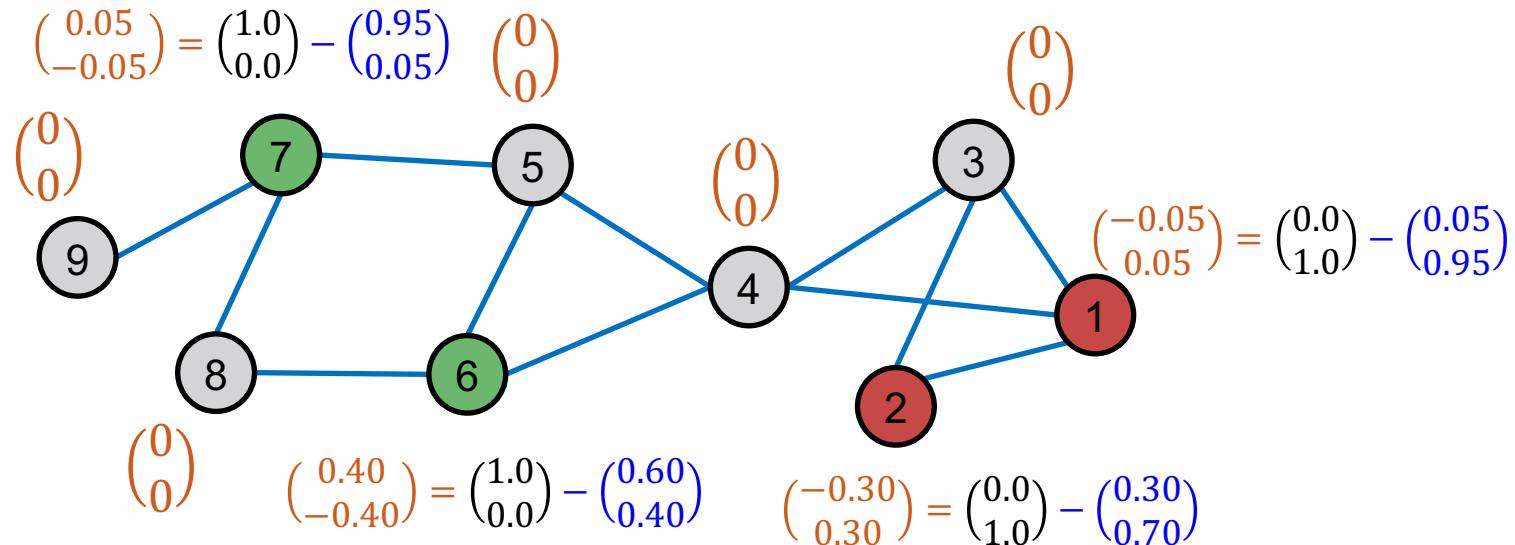
- The predicted soft labels may **not be smooth** over the graph.
- We need to smoothen the soft labels.



# C&S Post-Processing: Correct Step (1)

## ■ Correct step:

- Compute training errors of nodes.
  - **Training error:** Ground-truth label minus soft label.  
Defined as 0 for unlabeled nodes.

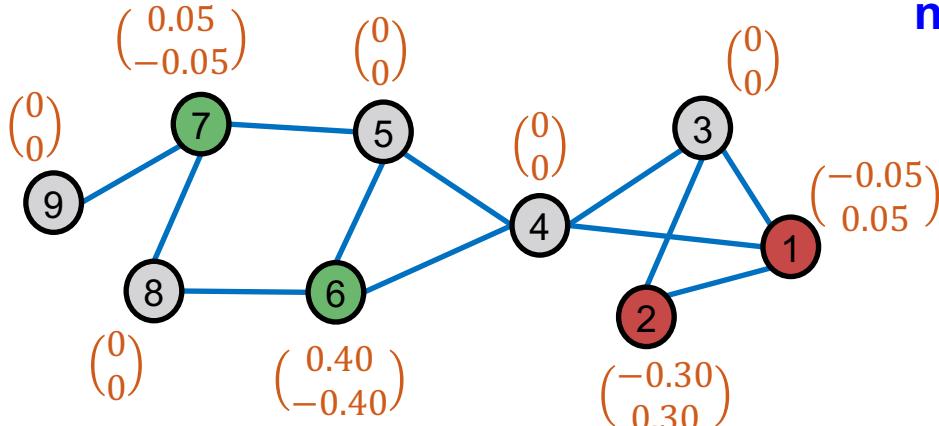


# C&S Post-Processing: Correct Step (2)

## ■ Correct step (contd.):

- Diffuse **training errors**  $E^{(0)}$  along the edges.
- Let  $A$  be the adjacency matrix,  $\tilde{A}$  be the **diffusion matrix** (defined in the next slide).
- $E^{(t+1)} \leftarrow (1 - \boxed{\alpha}) \cdot E^{(t)} + \alpha \cdot \boxed{\tilde{A}E^{(t)}}.$ 
  - Similar to PageRank.

Diffuse training errors along the edges  
**Assumption: errors are similar for nearby nodes**

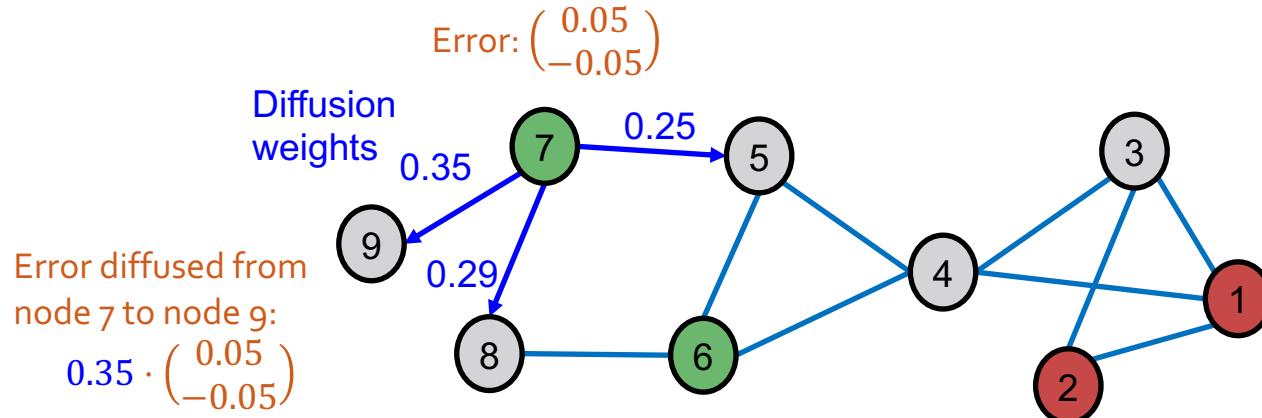


Initial  
training  
error  
matrix

$$E^{(0)} = \begin{pmatrix} -0.05 & 0.05 \\ -0.30 & 0.30 \\ 0 & 0 \\ 0 & 0 \\ 0.40 & -0.40 \\ 0.05 & -0.05 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}$$

# Diffusion Matrix $\hat{A}$

- Normalized diffusion matrix  $\tilde{A} \equiv D^{-1/2} A D^{-1/2}$ 
  - Add self-loop to the adjacency matrix  $A$ , i.e.,  $A_{ii} = 1$ .
  - Let  $D \equiv \text{Diag}(d_1, \dots, d_N)$  be the degree matrix.
  - See [Zhu et al. ICML 2013](#) for details.

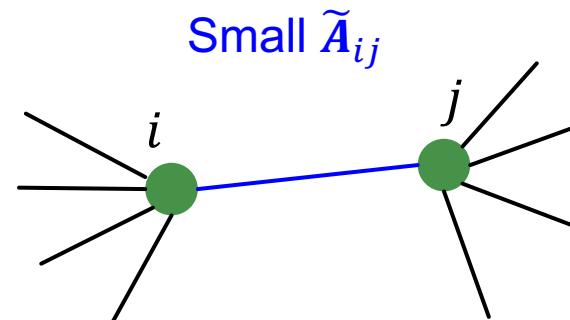
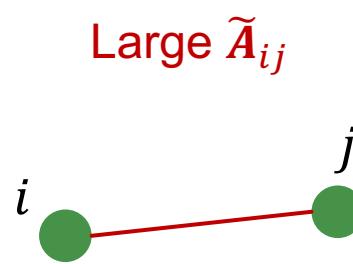


# Theoretical Motivation for $\tilde{A}$

- Normalized diffusion matrix  $\tilde{A} \equiv D^{-1/2}AD^{-1/2}$
- All the eigenvalues  $\lambda$ 's are in the range of [-1,1].
  - Eigenvector for  $\lambda = 1$  is  $D^{1/2}\mathbf{1}$  ( $\mathbf{1}$  is an all-one vector).
    - Proof:  $\tilde{A}D^{-1/2}\mathbf{1} = D^{-1/2}AD^{-1/2}D^{1/2}\mathbf{1} = D^{-1/2}A\mathbf{1} = D^{-1/2}D\mathbf{1} = 1 \cdot D^{1/2}\mathbf{1}$ .
  - The power of  $\tilde{A}$  (i.e.,  $\tilde{A}^K$ ) is well-behaved for any  $K$ .
    - The eigenvalues of  $\tilde{A}^K$  are always in the range of [-1,1].
    - The largest eigenvalue is always 1.

# Intuition for $\tilde{A}$

- If  $i$  and  $j$  are connected, the weight  $\tilde{A}_{ij}$  is  $\frac{1}{\sqrt{d_i}\sqrt{d_j}}$
- Intuition:
  - **Large** if  $i$  and  $j$  are connected only with each other (no other nodes are connected to  $i$  and  $j$ ).
  - **Small** if  $i$  and  $j$  are connected also connected with many other nodes.

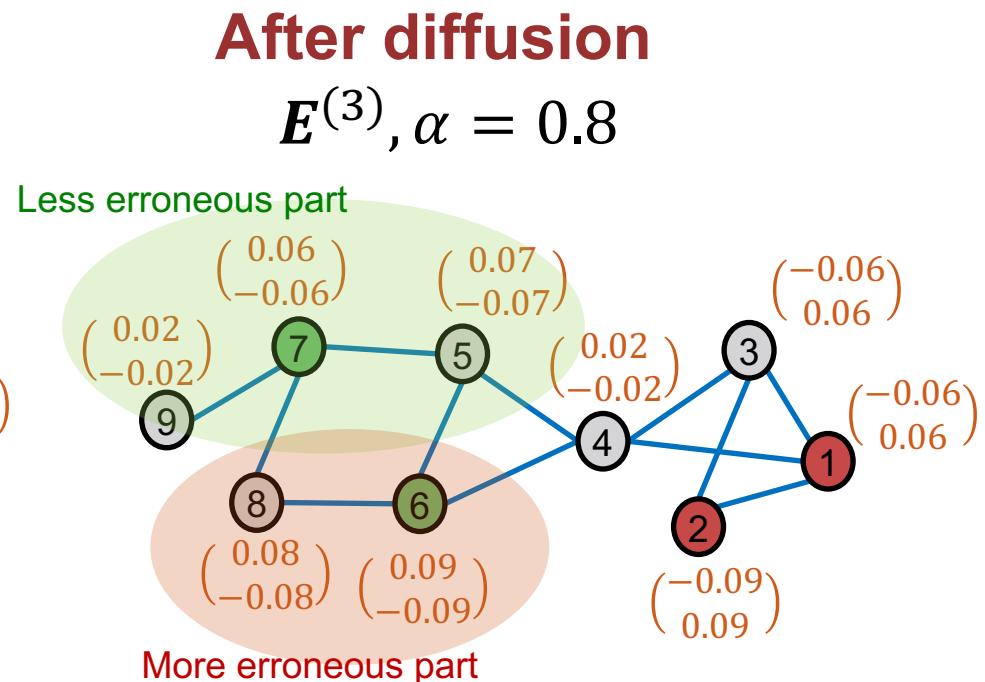
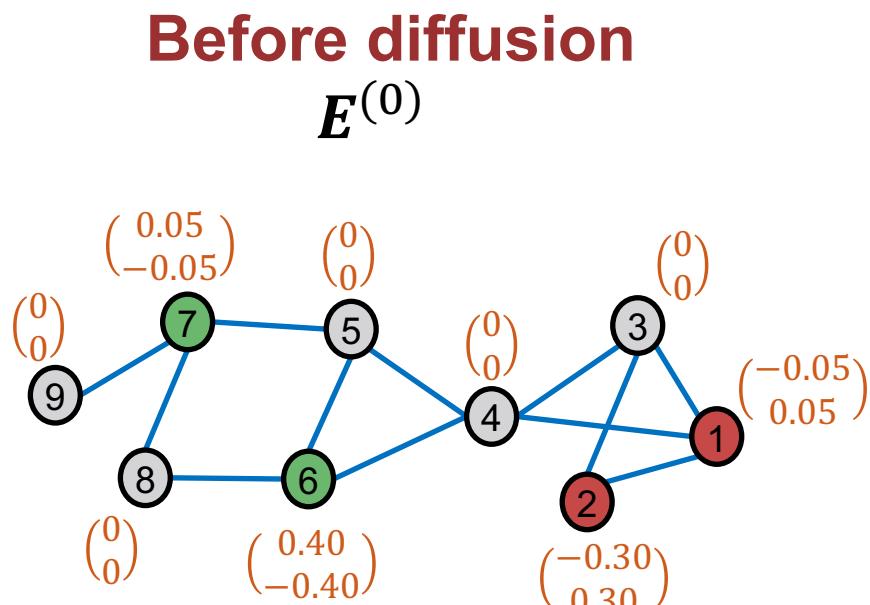


# C&S Post-Processing: Correct Step (3)

## Diffusion of training errors:

$$E^{(t+1)} \leftarrow (1 - \alpha) \cdot E^{(t)} + \alpha \cdot \tilde{A}E^{(t)}$$

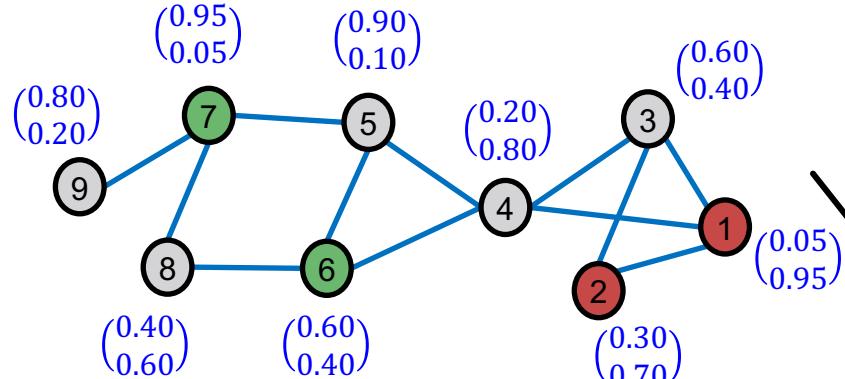
**Assumption:** Prediction errors are similar for nearby nodes.



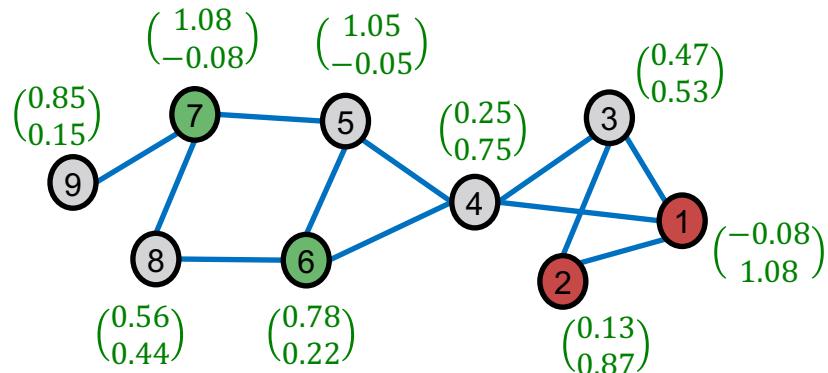
# C&S Post-Processing: Correct Step (4)

- Add the scaled diffused training errors into the predicted soft labels

Soft labels



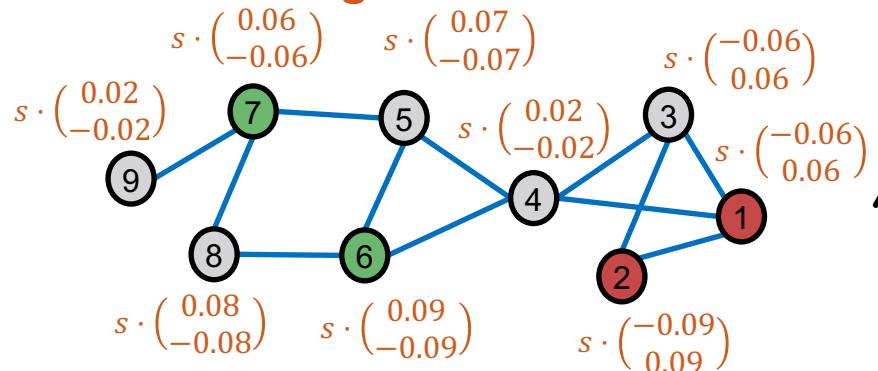
Output after the correct step ( $s = 2$ )



+

Scale by  $s$   
(hyper-parameter)

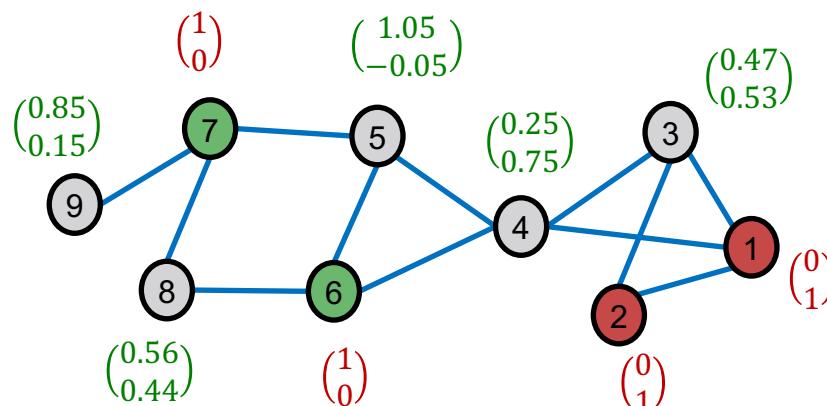
Diffused training errors



# C&S Post-Processing: Smooth Step

- Smoothen the corrected soft labels along the edges.
  - **Assumption:** Neighboring nodes tend to share the same labels.
  - **Note:** For training nodes, we use the **ground-truth hard labels** instead of the soft labels.

Input to the smooth step:



# C&S Post-Processing: Smooth Step (1)

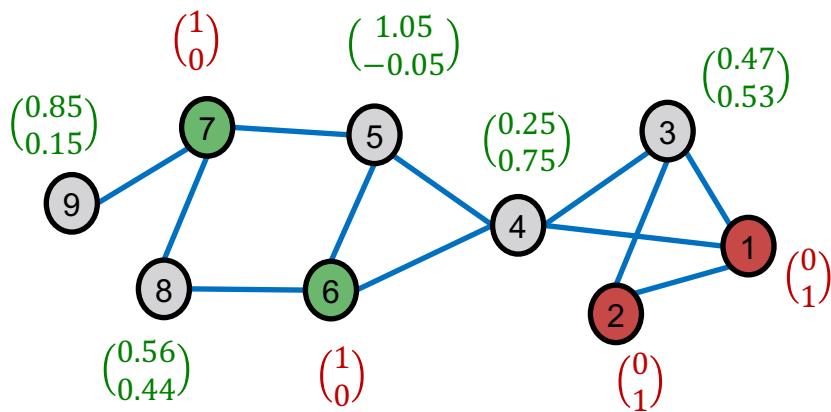
## ■ Smooth step:

- Diffuse label  $Z^{(0)}$  along the graph structure.

$$Z^{(t+1)} \leftarrow (1 - \boxed{\alpha}) \cdot Z^{(t)} + \alpha \cdot \boxed{\tilde{A}Z^{(t)}}.$$

Hyper-parameter

Diffuse labels along the edges



Corrected  
label  
matrix

$$Z^{(0)} = \begin{pmatrix} 0 & 1 \\ 0 & 1 \\ 0.47 & 0.53 \\ 0.25 & 0.75 \\ 1.05 & -0.05 \\ 1 & 0 \\ 1 & 0 \\ 0.56 & 0.44 \\ 0.85 & 0.15 \end{pmatrix}$$

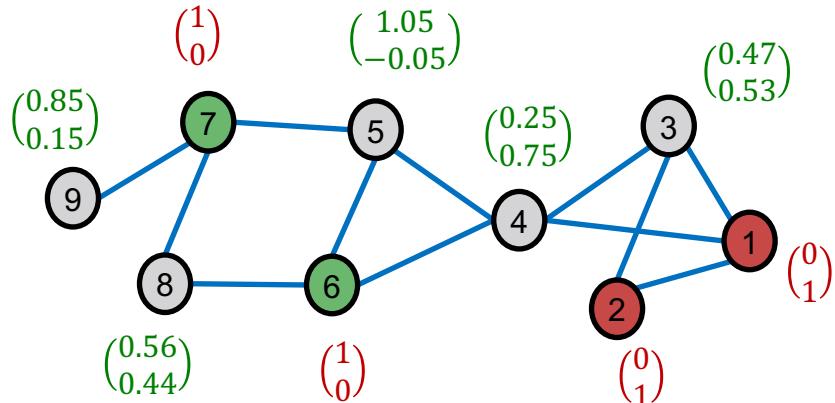
# C&S Post-Processing: Correct Step (2)

## ■ Smooth step:

$$\mathbf{Z}^{(t+1)} \leftarrow (1 - \alpha) \cdot \mathbf{Z}^{(t)} + \alpha \cdot \tilde{\mathbf{A}}\mathbf{Z}^{(t)}$$

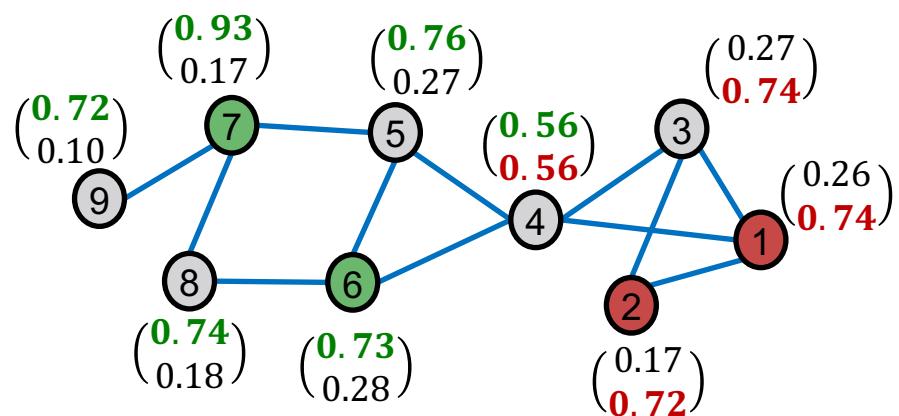
Before smoothing

$\mathbf{Z}^{(0)}$



After smoothing

$\mathbf{Z}^{(3)}, \alpha = 0.8$



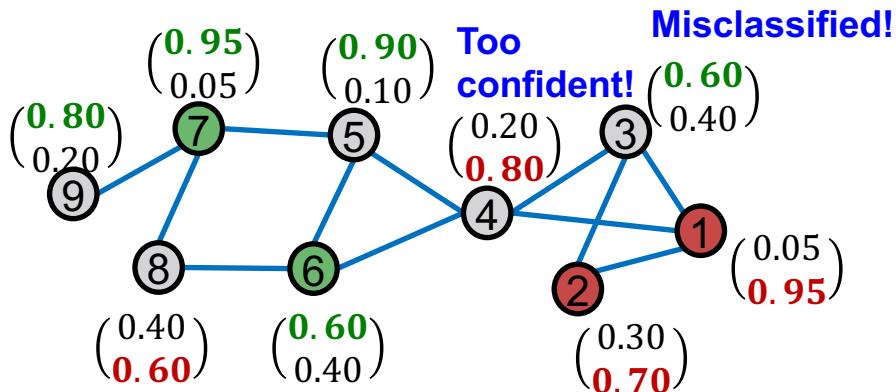
The final class prediction of C&S is the class with the maximum  $\mathbf{Z}^{(3)}$  score.

**Note:** The  $\mathbf{Z}^{(3)}$  scores do not have direct probabilistic interpretation (e.g., not sum to 1 for each node), but larger scores indicate the classes are more likely.

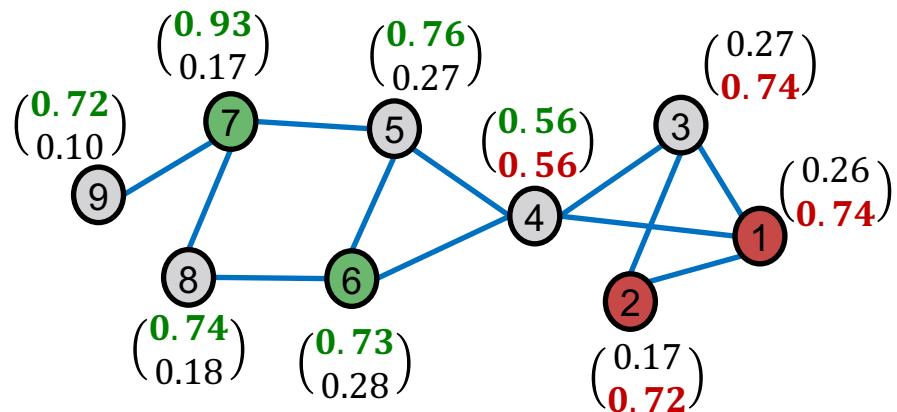
# C&S: Toy Example Summary

- Our toy example shows that C&S successfully improves base model performance using graph structure.

Prediction of the base model



After C&S



# C&S on a Real-World Dataset

- C&S significantly improves the performance of the base model (MLP).
- C&S outperforms Smooth-only (no correct step) baseline.

Method	Classification accuracy (%) on ogbn-products dataset
MLP (base model)	63.41
MLP + smooth only	80.34
<b>MLP + C&amp;S</b>	<b>84.18</b>

# Correct & Smooth: Summary

- Correct & Smooth (C&S) **uses graph structure to post-process** the soft node labels predicted by any base model.
- **Correction step:** Diffuse and correct for the training errors of the base predictor.
- **Smooth step:** Smoothen the prediction of the base predictor.
- C&S achieves strong performance on semi-supervised node classification.

# Summary

- We learned how to leverage correlation in graphs to make prediction on nodes.

- Key techniques:

- Relational classification
- Iterative classification
- Correct & Smooth

- Loopy belief propagation

-

may cause problem  
in graphs with cycles.

돌고로운 흐름 막기