Stanford CS224W: Message Passing and Node Classification

CS224W: Machine Learning with Graphs
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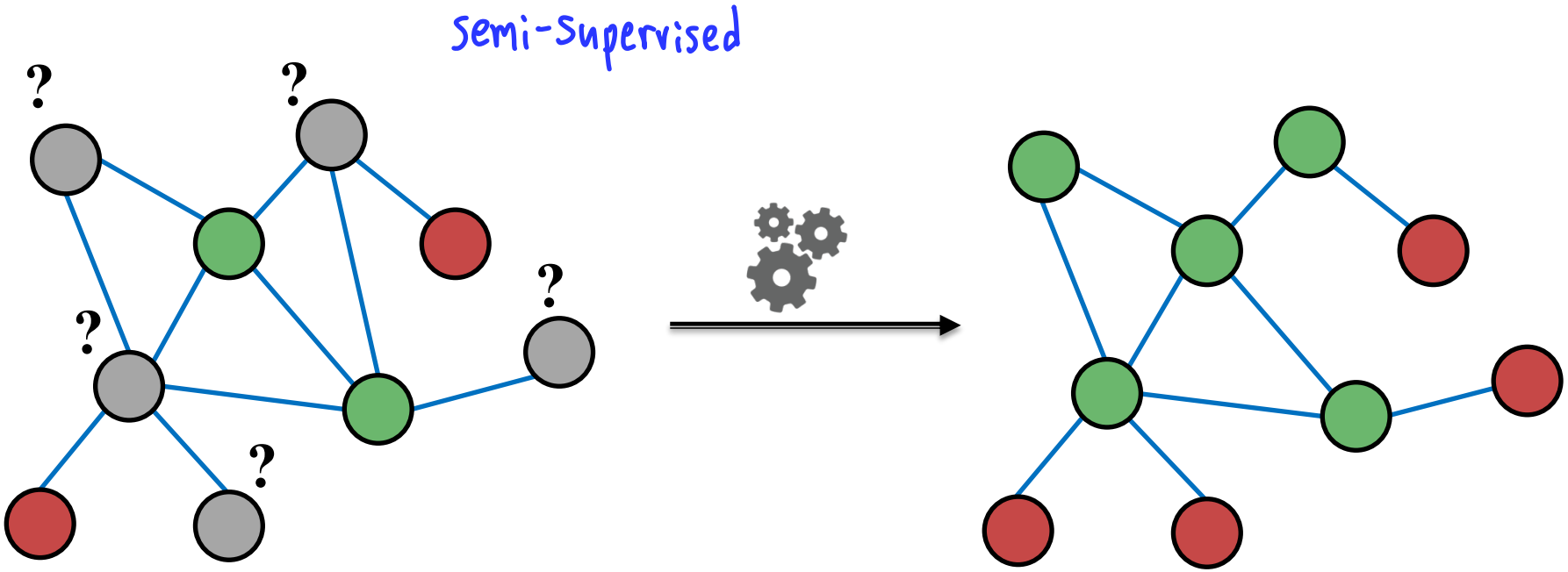
http://cs224w.stanford.edu

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

Outline

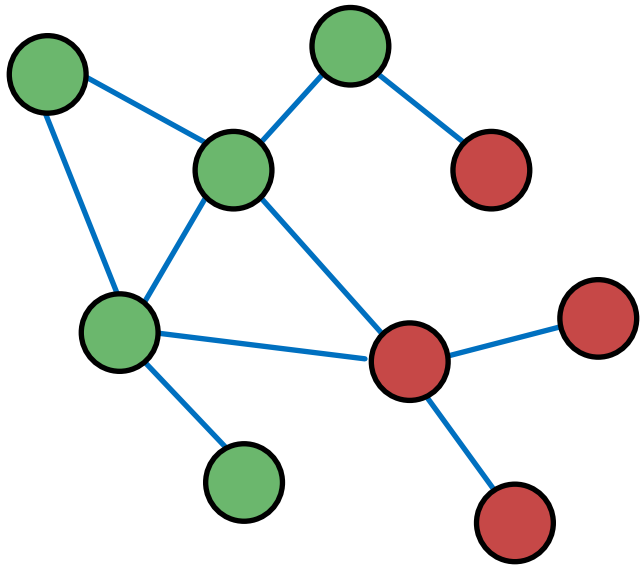
message passing framework

- **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 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**
  - **Belief propagation**

nodes where labels tend to be connected

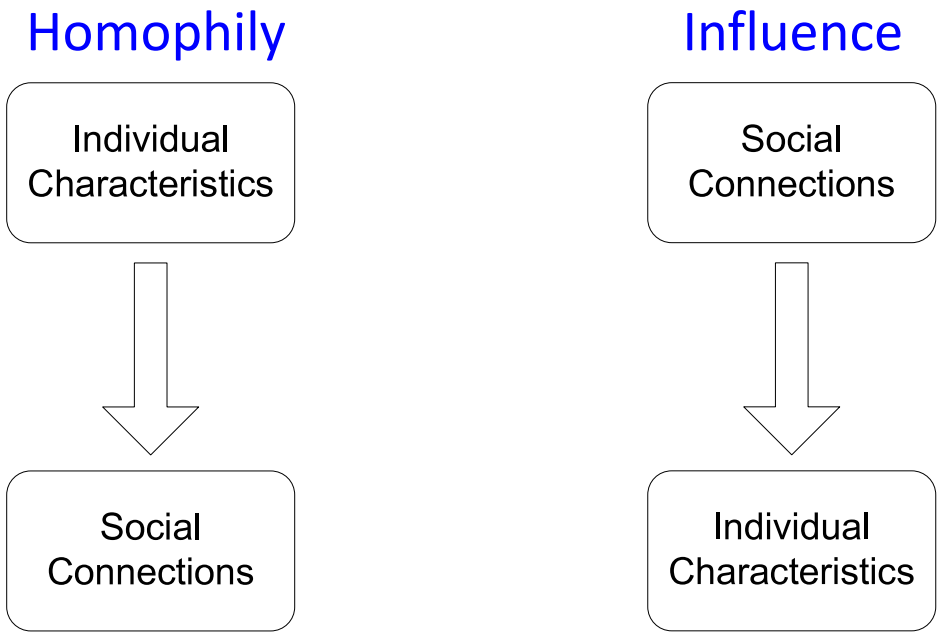
Correlations Exists in Networks

- Individual behaviors are **correlated** in the network
- **Correlation**: nearby nodes have the same color (belonging to the same class)



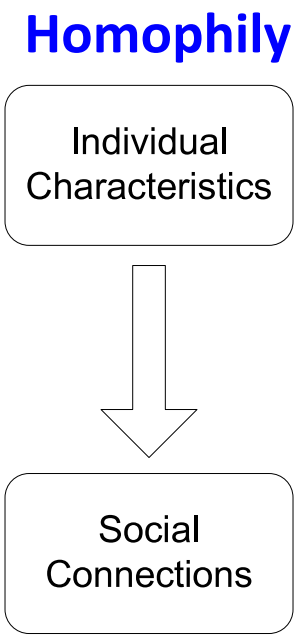
Correlations Exist in Networks

- **Main types of dependencies that lead to correlation:**



Homophily

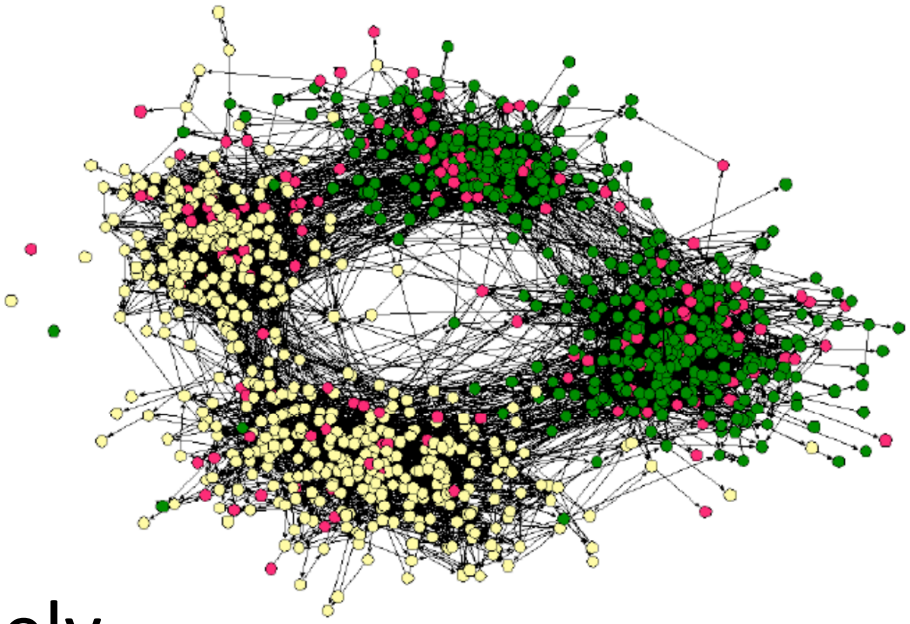
- **Homophily**: The tendency of individuals to associate and bond with similar others
  - *"Birds of a feather flock together"*
  - It has been observed in a vast array of network studies, based on a variety of attributes (e.g., age, gender, organizational role, etc.)
  - **Example**: Researchers who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



Homophily: Example

Example of homophily

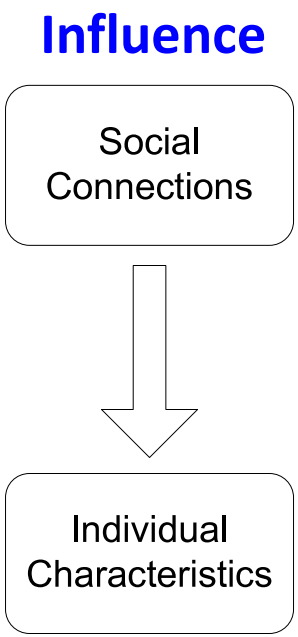
- Online social network
  - Nodes = people
  - Edges = friendship
  - Node color = interests (sports, arts, etc.)
- People with the same interest are more closely connected due to homophily



(Easley and Kleinberg, 2010)

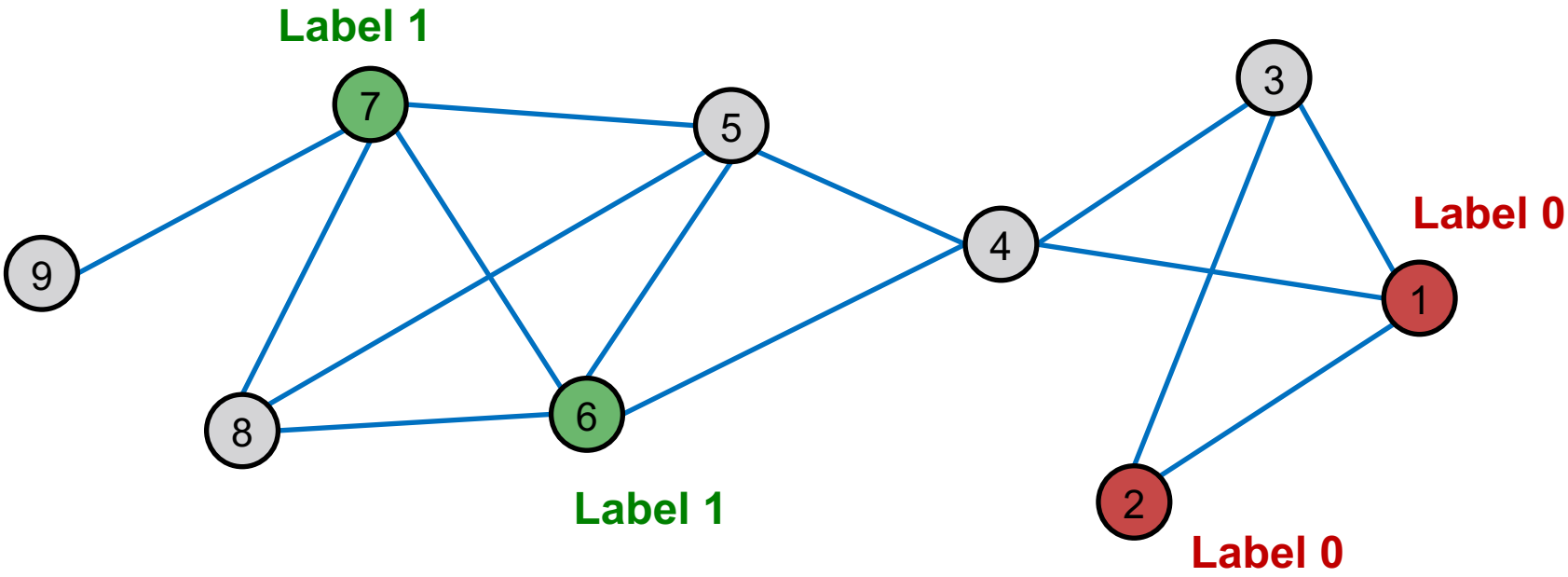
Influence

- **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!



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?

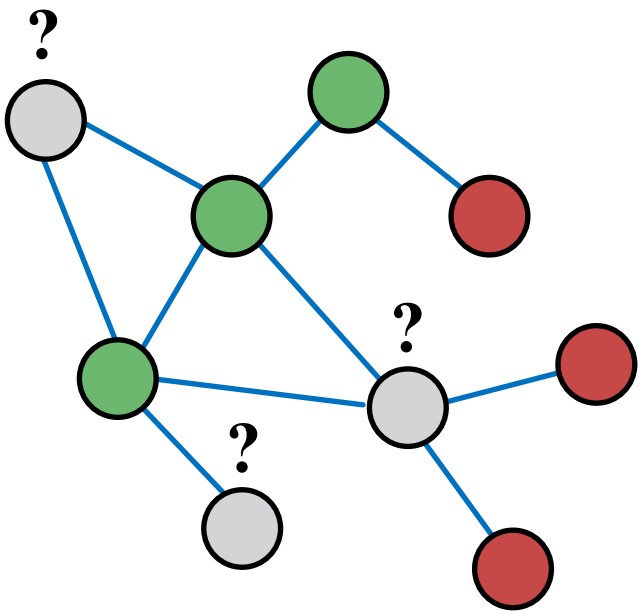
Motivation (1)

- **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:
  1. Features of v
  2. Labels of the nodes in v's neighborhood
  3. Features of the nodes in v's neighborhood

Semi-supervised Learning (1)



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 $\boldsymbol{A}$ be a $n \times n$ adjacency matrix over n nodes
- Let $\mathrm{Y} = \{0, 1\}^n$ be a vector of **labels**:
  - $\mathrm{Y}_v = 1$ belongs to Class 1
  - $\mathrm{Y}_v = 0$ 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**

Approach: Collective Classification

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

Collective Classification Overview (1)

- **Intuition**: Simultaneous classification of interlinked nodes using correlations
- Probabilistic framework
- Markov Assumption: *the label Y_v of one node v depends on the labels of its neighbors N_v*

deg. 1 neighborhood

$$P(Y_v) = P(Y_v|N_v)$$

- Collective classification involves 3 steps:

Local Classifier	Relational Classifier	Collective Inference
• Assign initial labels	• Capture correlations between nodes	• Propagate correlations through network

Collective Classification Overview (2)

1st Local Classifier

- Assign initial labels

2nd Relational Classifier

- Capture correlations between nodes

3rd Collective Inference

- Propagate correlations through network

Local Classifier: Used for initial label assignment

- Predicts label based on node attributes/features
- Standard classification task
- Does not use network information

apply only once, to give initial labels to the grey nodes at beginning

Relational Classifier: Capture correlations

- Learns a classifier to label one node based on the labels and/or attributes of its neighbors
- This is where network information is used

Collective Inference: Propagate the correlation

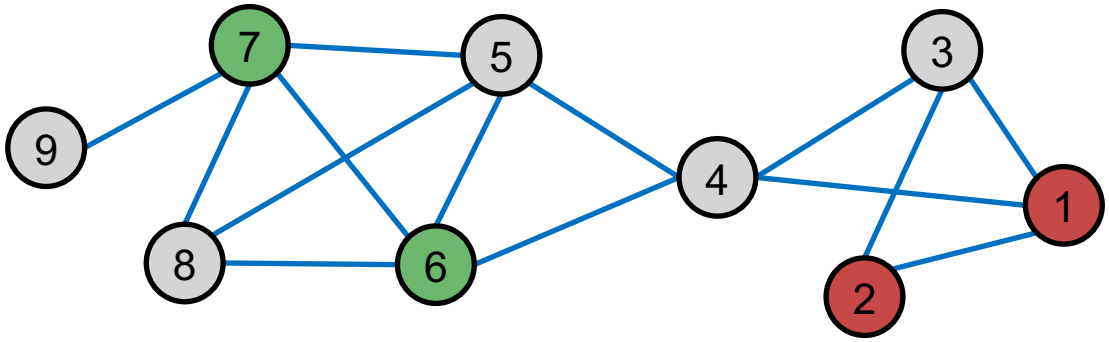
- Apply relational classifier to each node iteratively
- Iterate until the inconsistency between neighboring labels is minimized
- Network structure affects the final prediction

predictions are going to converge & stabilize

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

$P(Y_v) = ?$



Overview of What is Coming

partially labeled

- We focus on semi-supervised node classification
- Intuition is based on **homophily**: Similar nodes are typically close together or directly connected
- **Three techniques we will introduce:**
  - **Relational classification**
  - **Iterative classification**
  - **Belief propagation**

Stanford CS224W: Relational Classification and Iterative Classification

CS224W: Machine Learning with Graphs
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Collective Classification Models

- **Relational classifiers**
- Iterative classification
- Loopy belief propagation

Probabilistic Relational Classifier (1)

- **Basic idea:** 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^* given label
- 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

use node labels & network structure

not use node attributes features

Probabilistic Relational Classifier (2)

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

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

normalization [0, 1]

$\sum_{(v,u)\in E} A_{v,u}$: adjacent to v; in-deg. of v

$P(Y_u = c)$: likelihood that v belongs to class c

$\sum_{(v,u)\in E} A_{v,u} \cdot P(Y_u = c)$: is average likelihood that v neighbors belong to c

  - 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

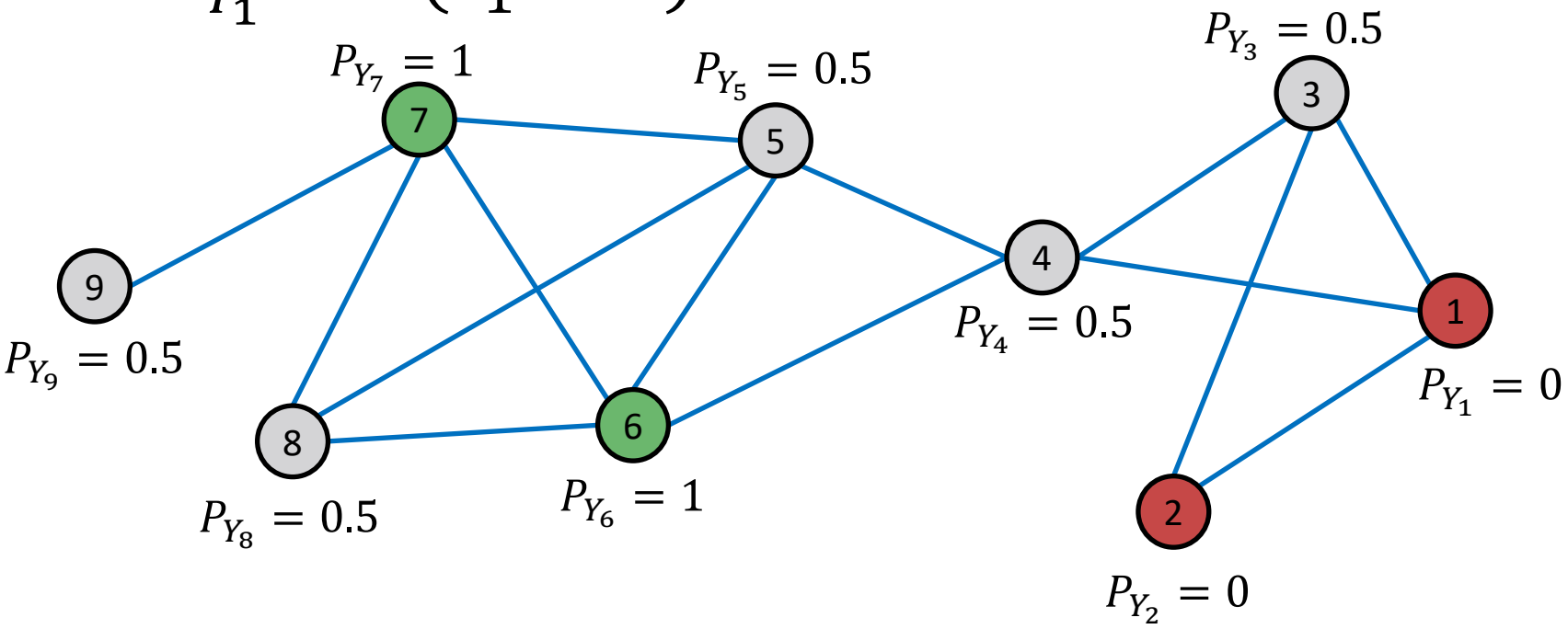
just node label & network information

Example: Initialization

Initialization:

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

Let $P_{Y_1} = P(Y_1 = 1)$

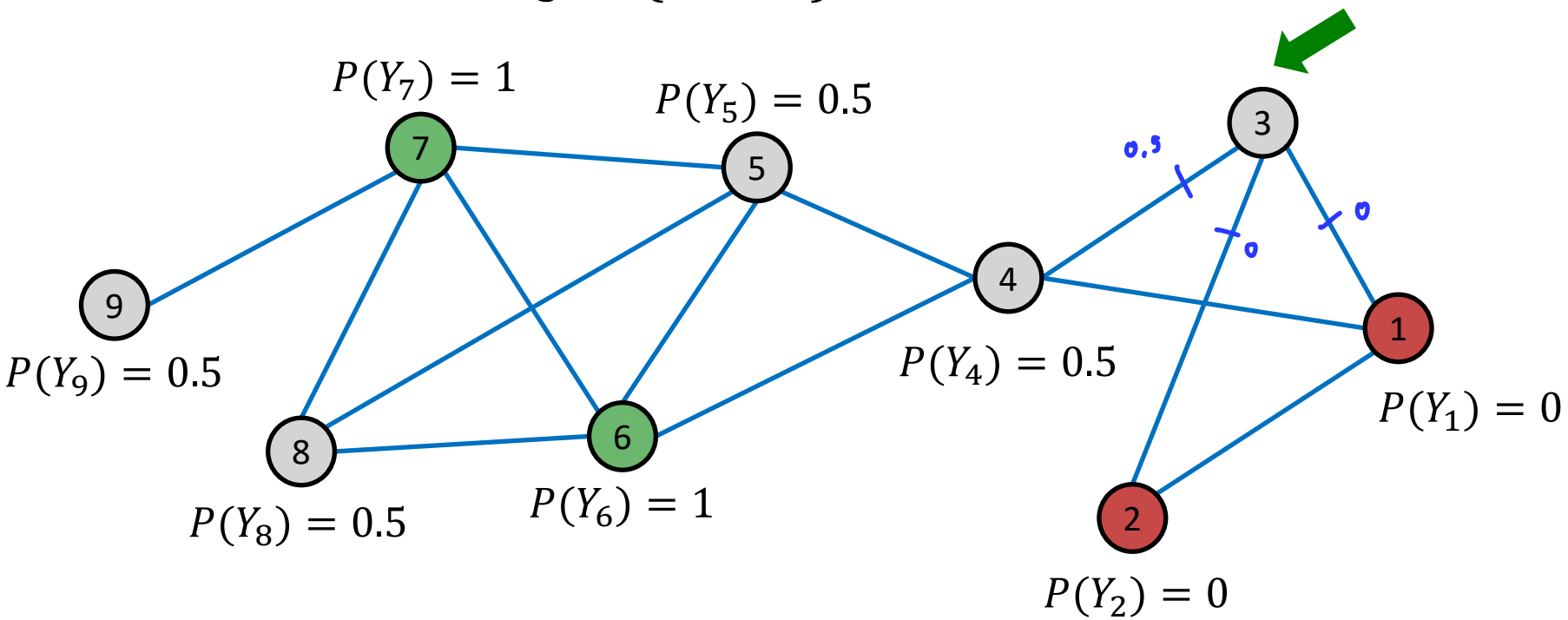


Example: 1st Iteration, Update Node 3

by node ID

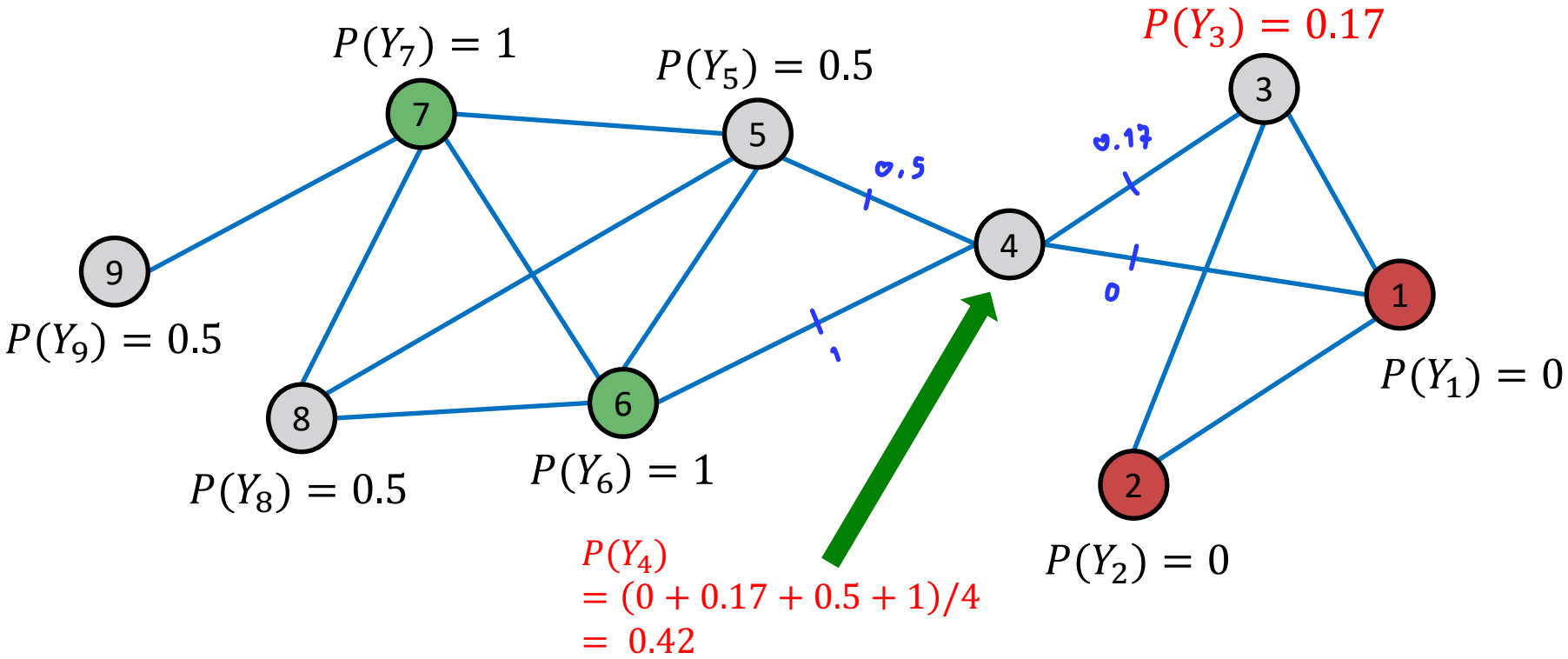
- Update for the 1st Iteration:
  - For node 3, $N_3 = \{1, 2, 4\}$

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



Example: 1st Iteration, Update Node 4

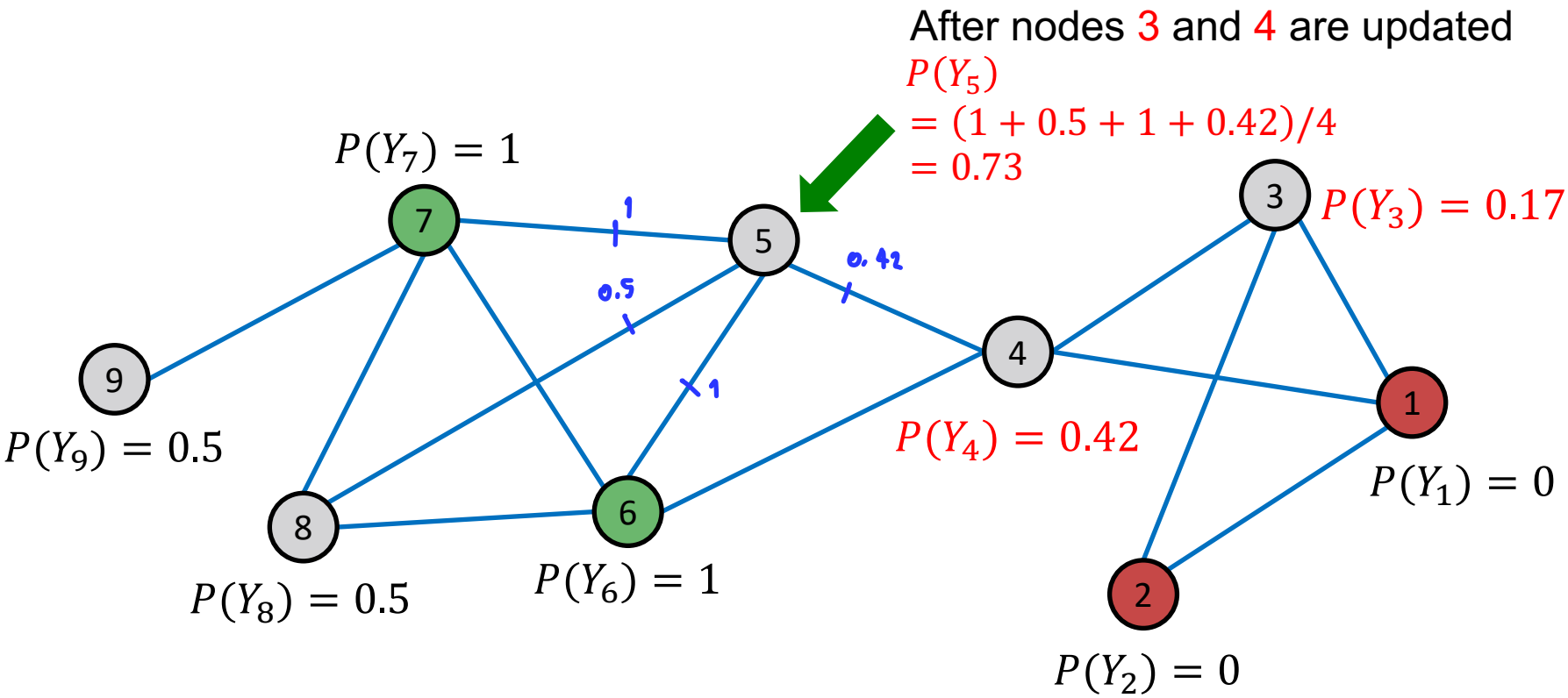
- Update for the 1st Iteration:
  - For node 4, $N_4 = \{1, 3, 5, 6\}$



After Node 3 is updated

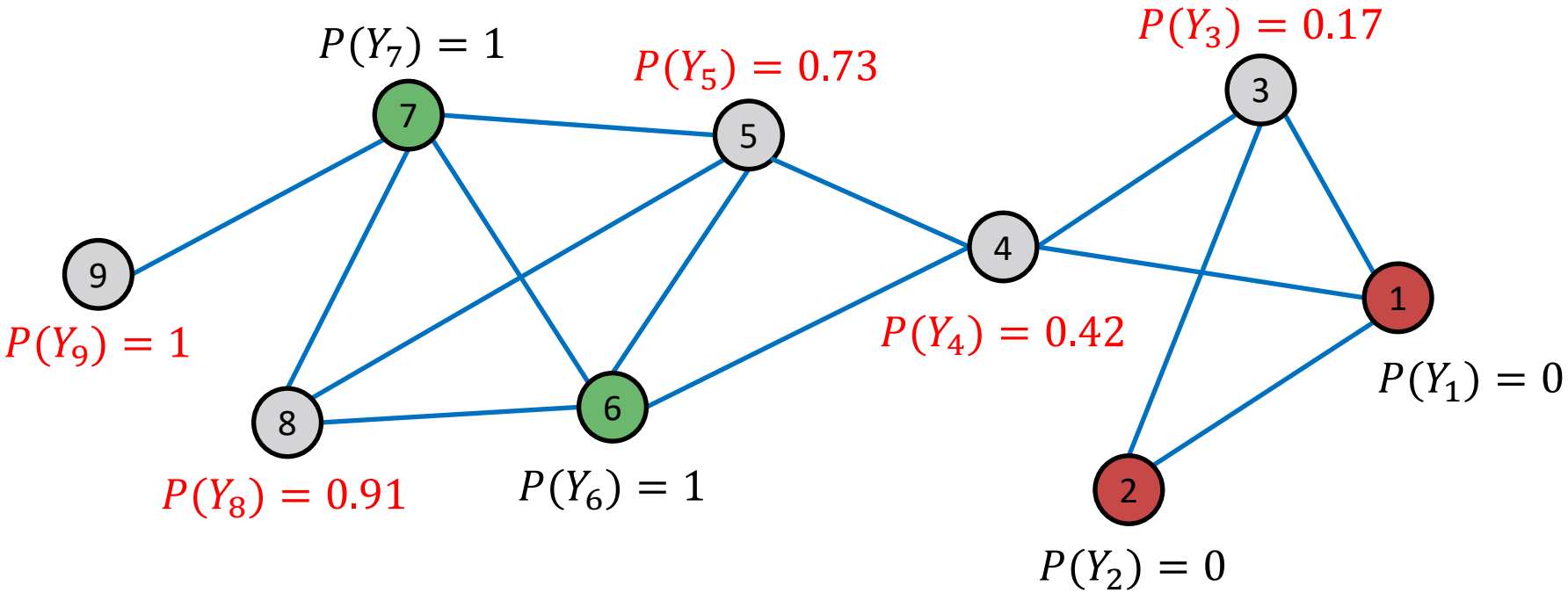
Example: 1st Iteration, Update Node 5

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



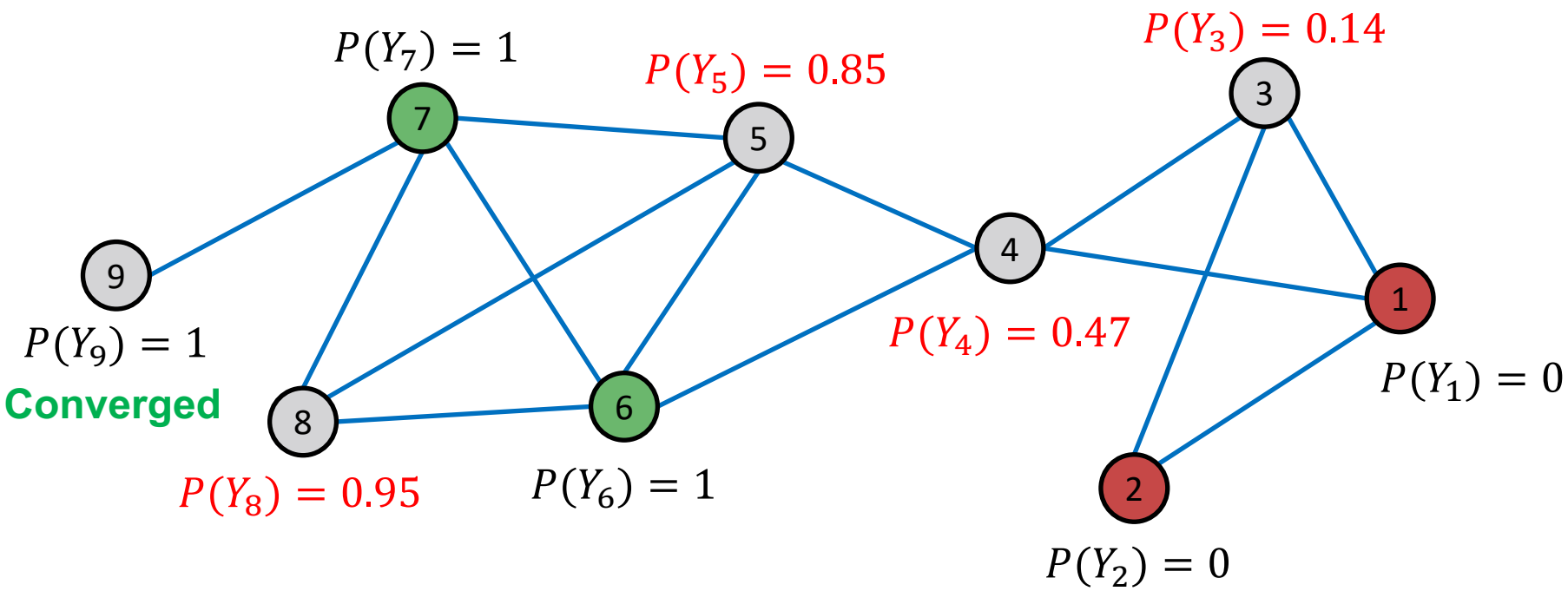
Example: After 1st Iteration

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



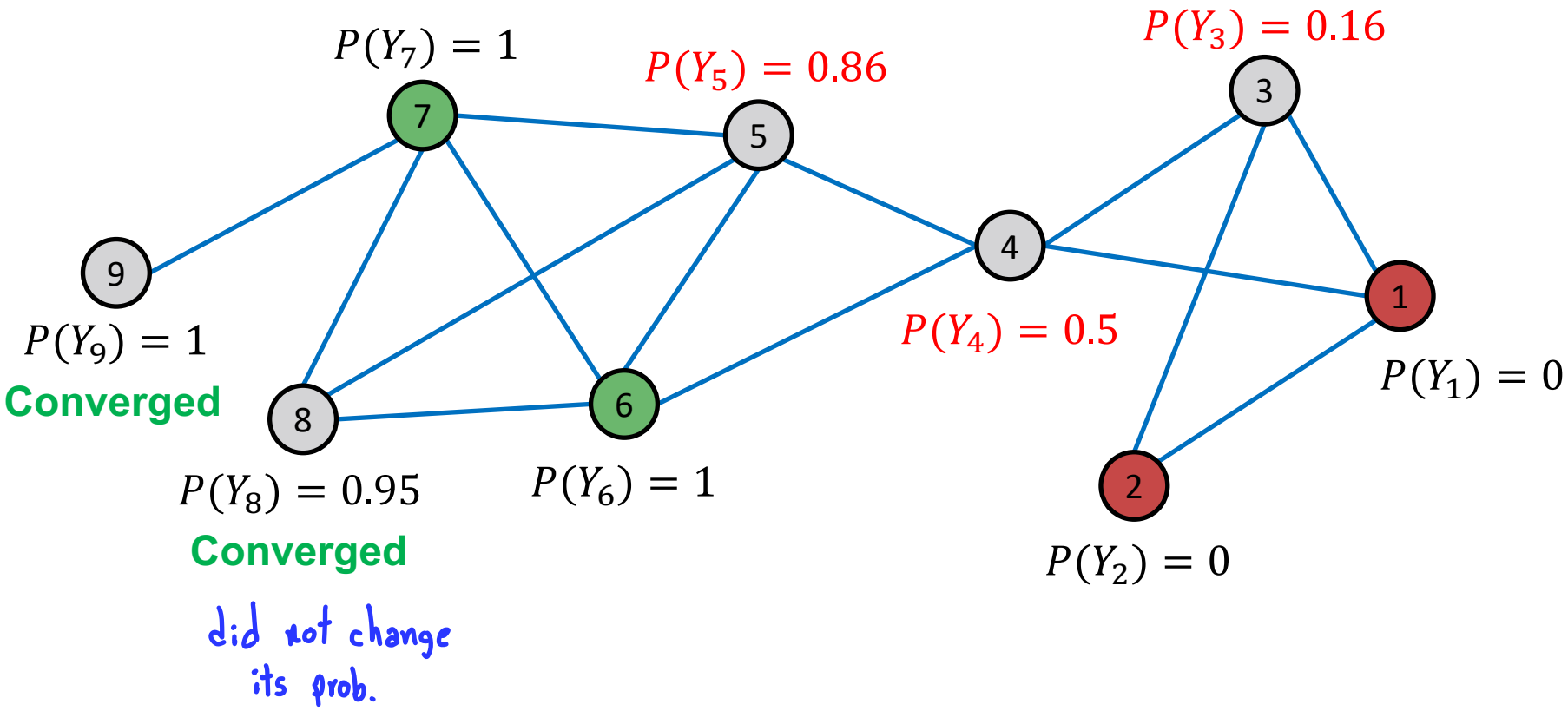
Example: After 2nd Iteration

After Iteration 2



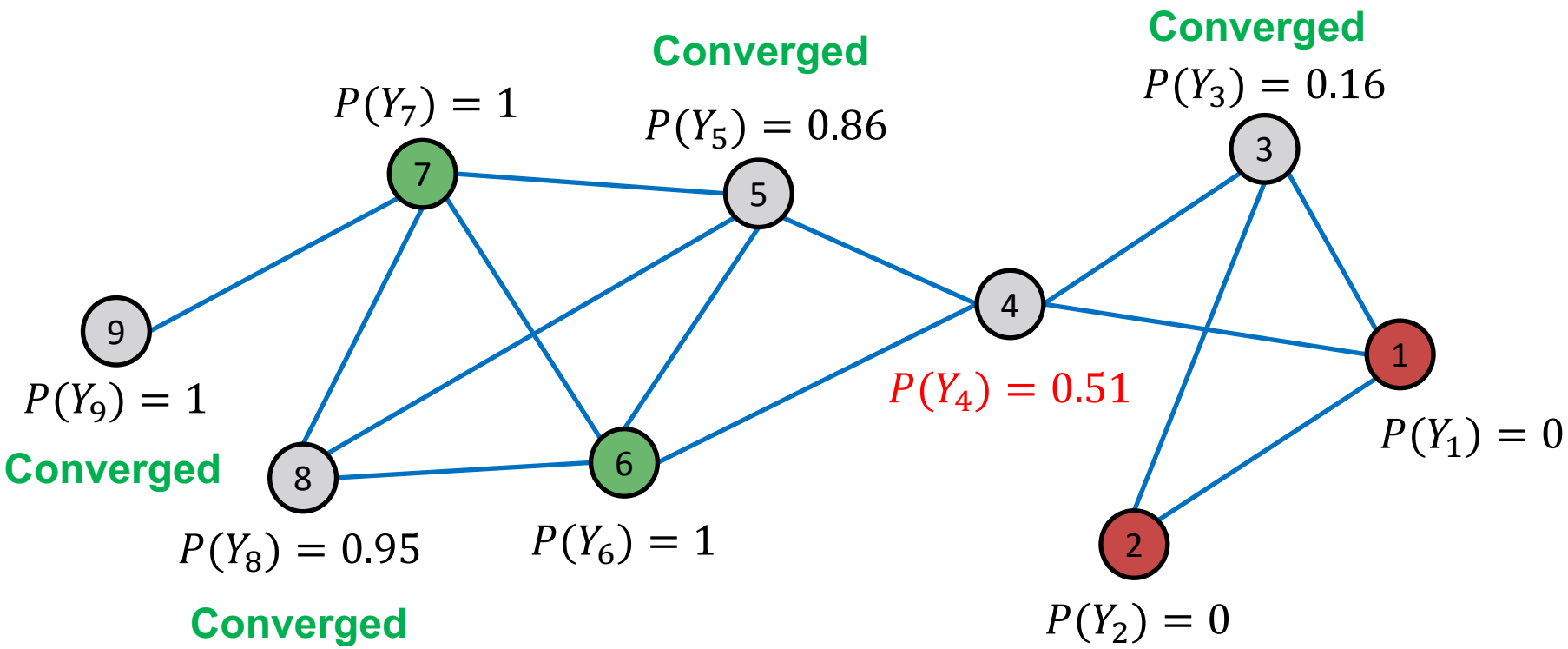
Example: After 3rd Iteration

After Iteration 3



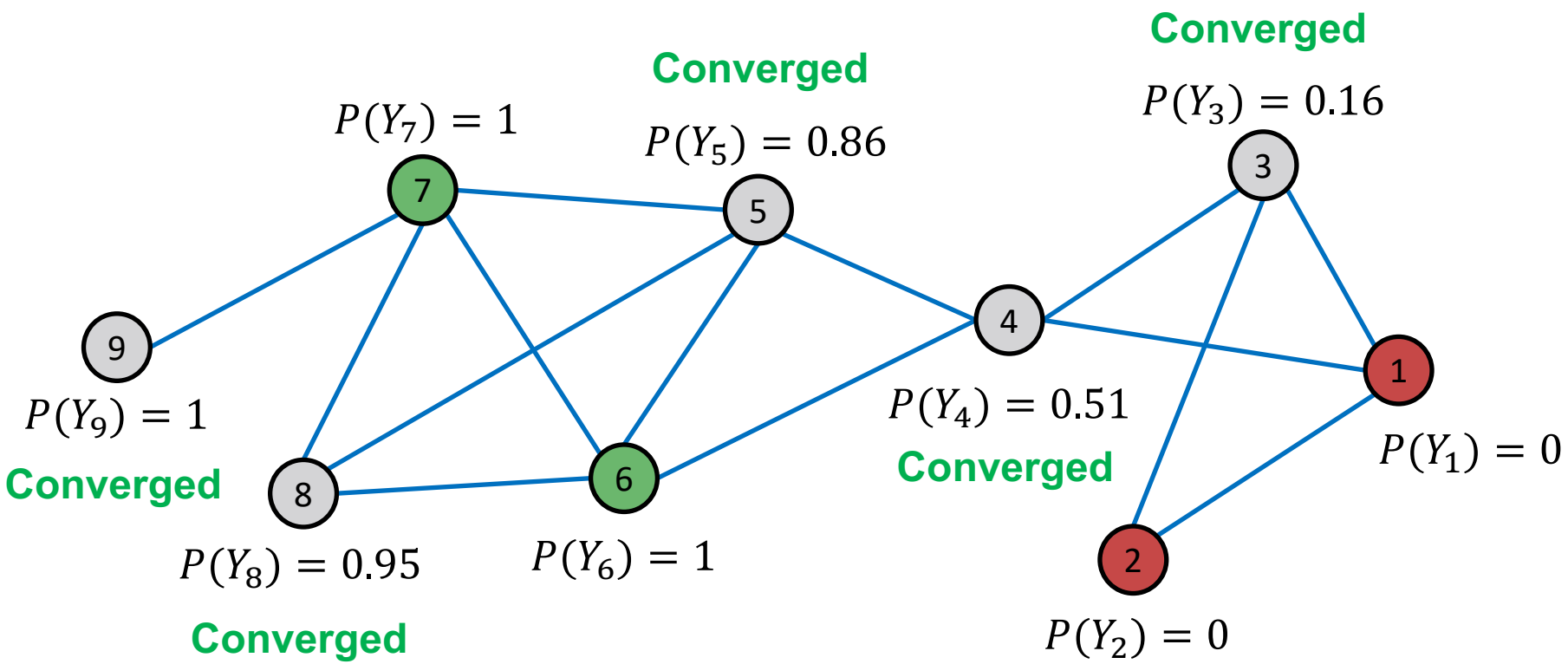
Example: After 4th Iteration

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 belong to class 0** ($P_{Y_v} < 0.5$)



Collective Classification Models

- Relational classifiers based on labels alone
- **Iterative classification** both node features & node labels
- Loopy belief propagation

Iterative Classification

- **Relational classifiers do 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 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:**

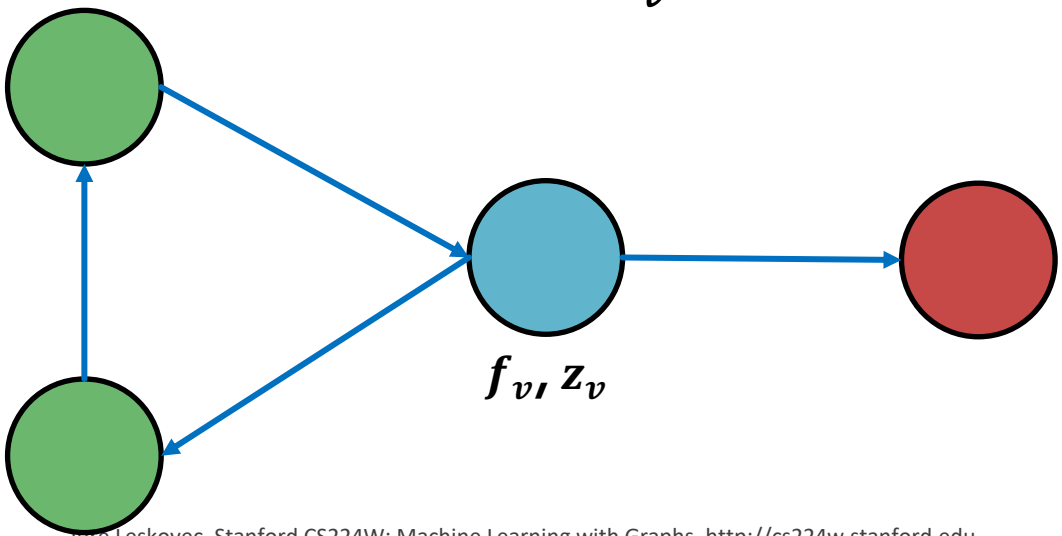
① $\phi_1(f_v)$ = Predict node label based on node feature vector f_v

② $\phi_2(f_v, z_v)$ = Predict label based on node feature vector f_v and summary z_v of labels of v's neighbors.

Computing the Summary z_v

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

- Ideas: z_v = **vector**
  - 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

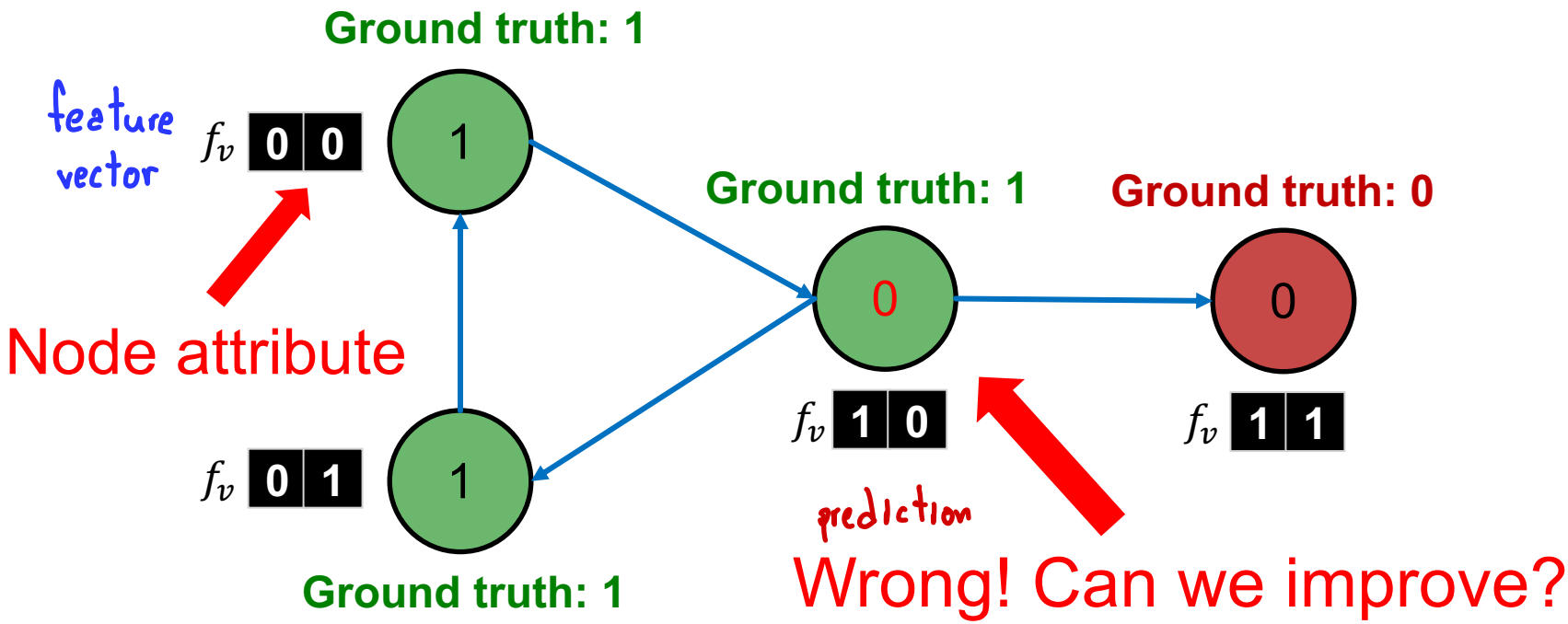
- **Phase 1: Classify based on node attributes alone**
  - On a **training set**, train classifier (e.g., linear classifier, neural networks, …):
  - ① $\phi_1(f_v)$ to predict Y_v based on f_v
  - ② $\phi_2(f_v, z_v)$ to predict Y_v based on f_v and summary z_v of labels of v's neighbors
- **Phase 2: Iterate till convergence**
  - On **test set**, set labels Y_v based on the classifier ϕ_1, compute z_v and predict the labels with ϕ_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 (ϕ_2)
  - Iterate until class labels stabilize or max number of iterations is reached
  - Note: Convergence is not guaranteed

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 2 binary features
- **Task:** Predict the topic of the webpage

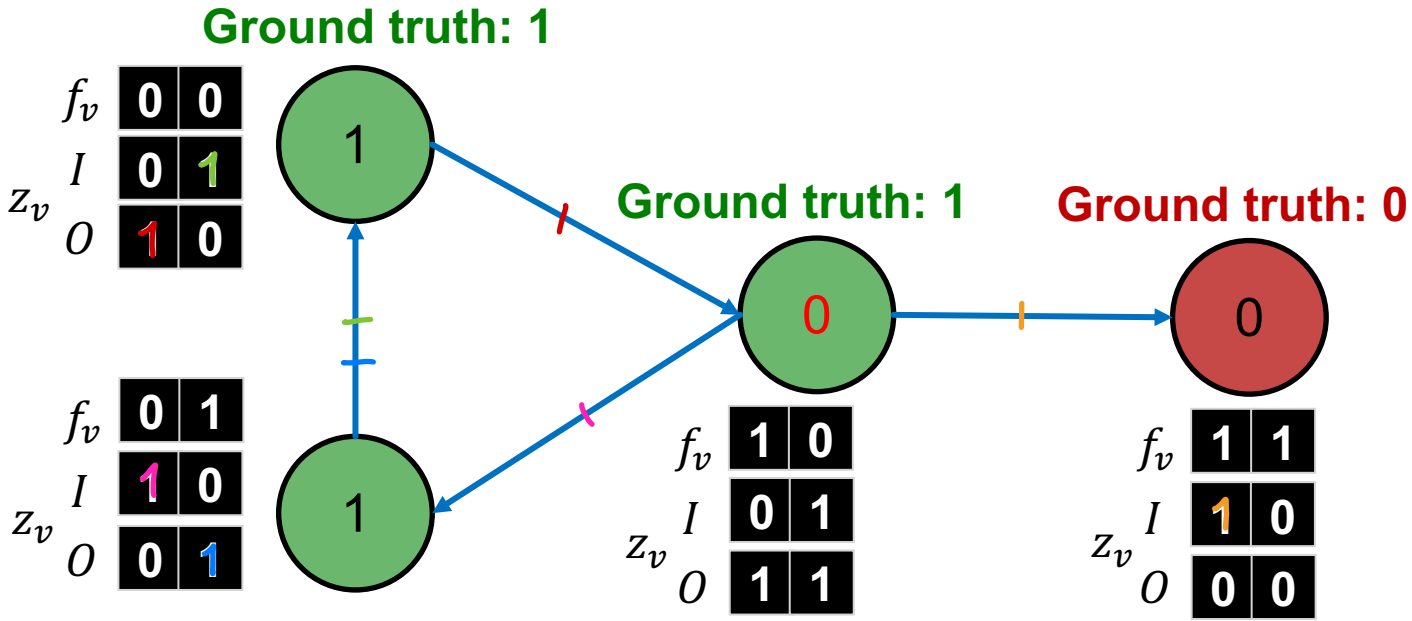
Example: Web Page Classification (2)

- Baseline: train a classifier (e.g., linear classifier) to classify pages based on binary node attributes. ϕ_1



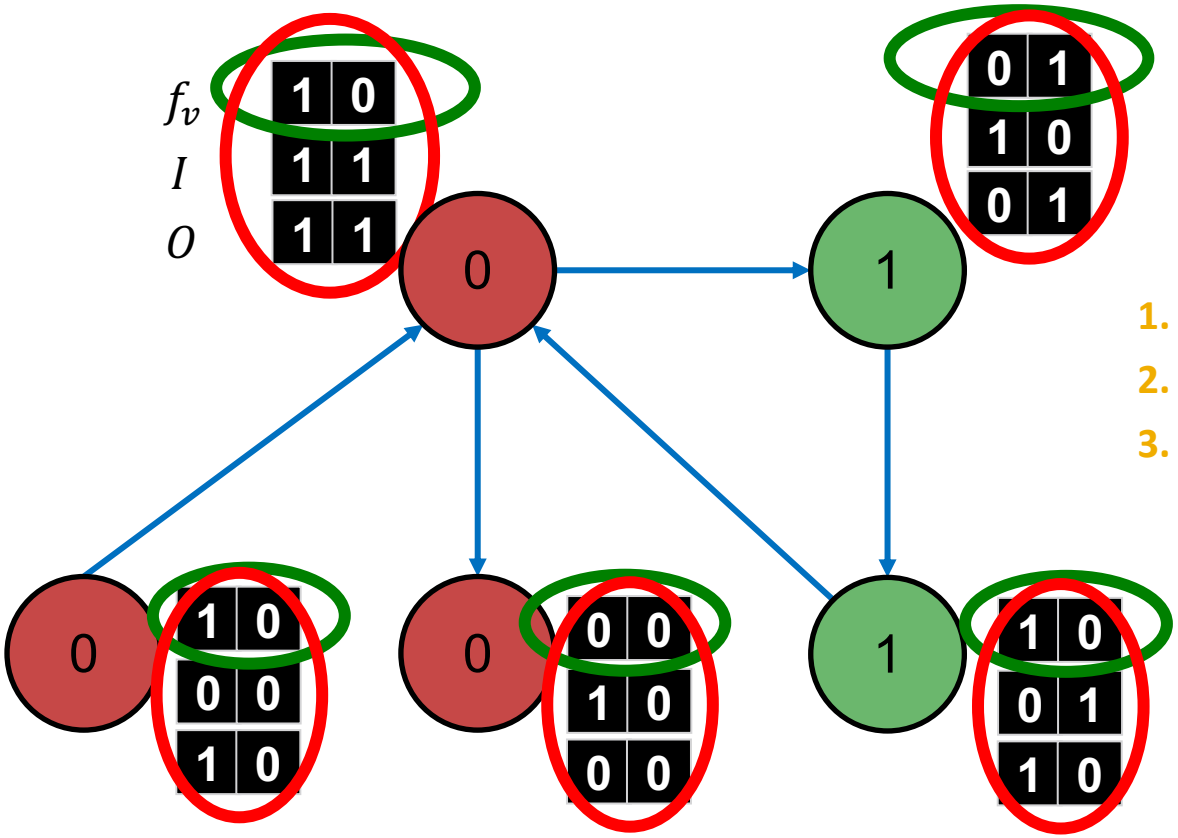
Example: Web Page Classification (3)

- Each node maintains vectors z_v of neighborhood labels:
  I = **Incoming** neighbor label information vector
  O = **Outgoing** neighbor label information vector
  as directed graph
- $I_0 = 1$ 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 a different **training set**, train two classifiers:
  - Node attribute vector only (green circles): ϕ_1
  - Node attribute and link vectors (red circles): ϕ_2

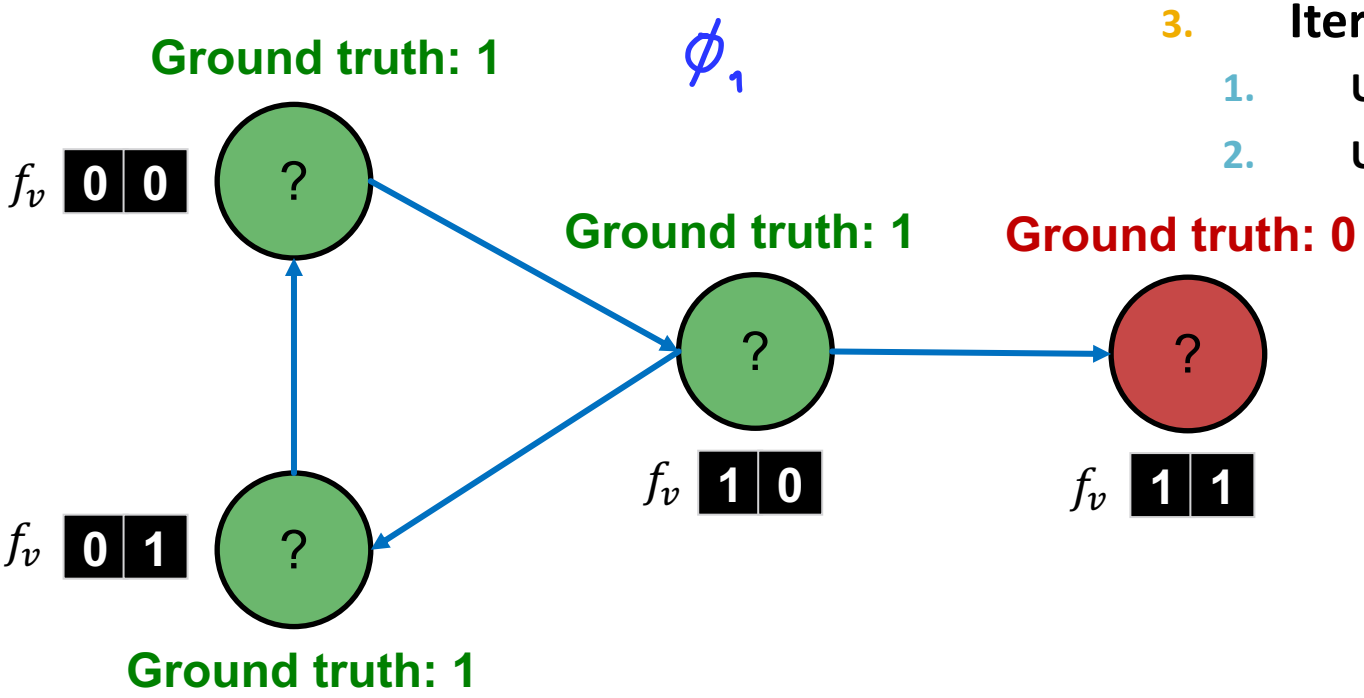


1. **Train classifier**
2. **Apply classifier to test set**
3. **Iterate**
   1. **Update relational features z_v**
   2. **Update label Y_v**

Iterative Classifier – Step 2

- On the **test set**:
  - Use trained node feature vector classifier ϕ_1 to set Y_v

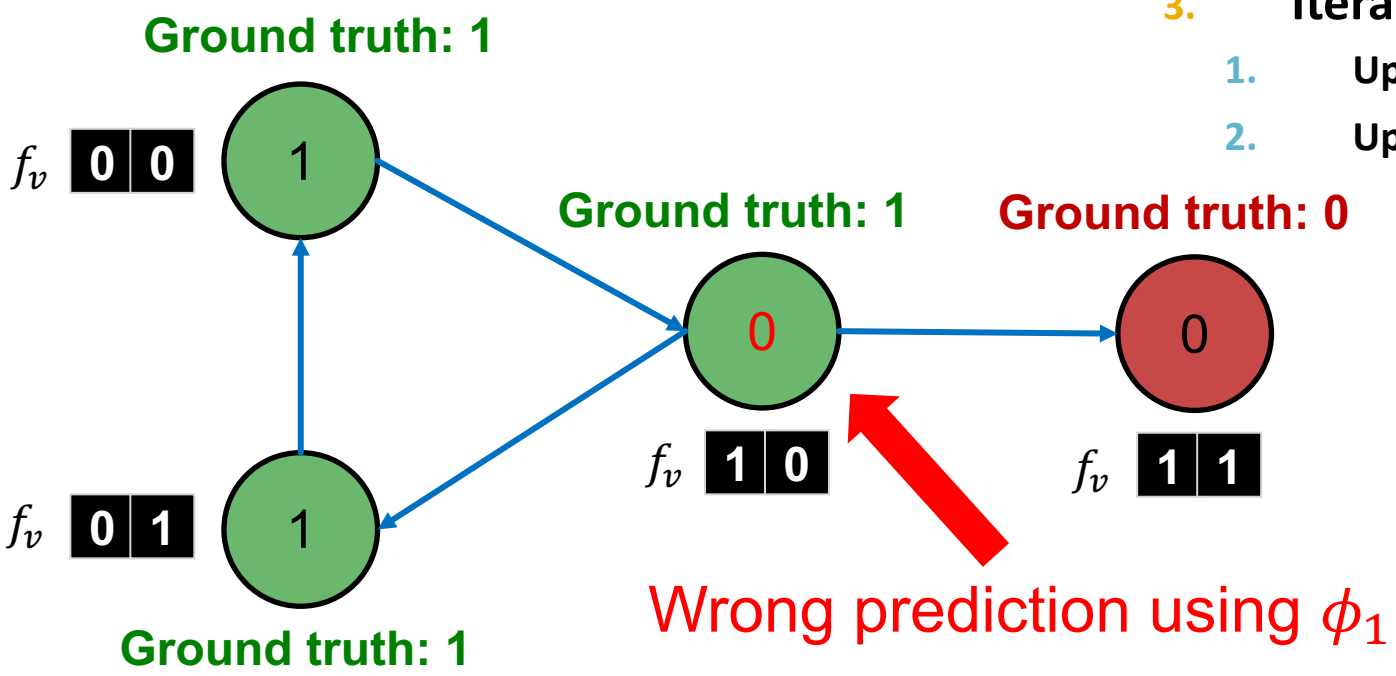
1. Train classifier
2. **Apply classifier to test set**
3. Iterate
   1. Update relational features z_v
   2. Update label Y_v



Iterative Classifier – Step 2

- On the **test set**:
  - Use trained node feature vector classifier ϕ_1 to set Y_v

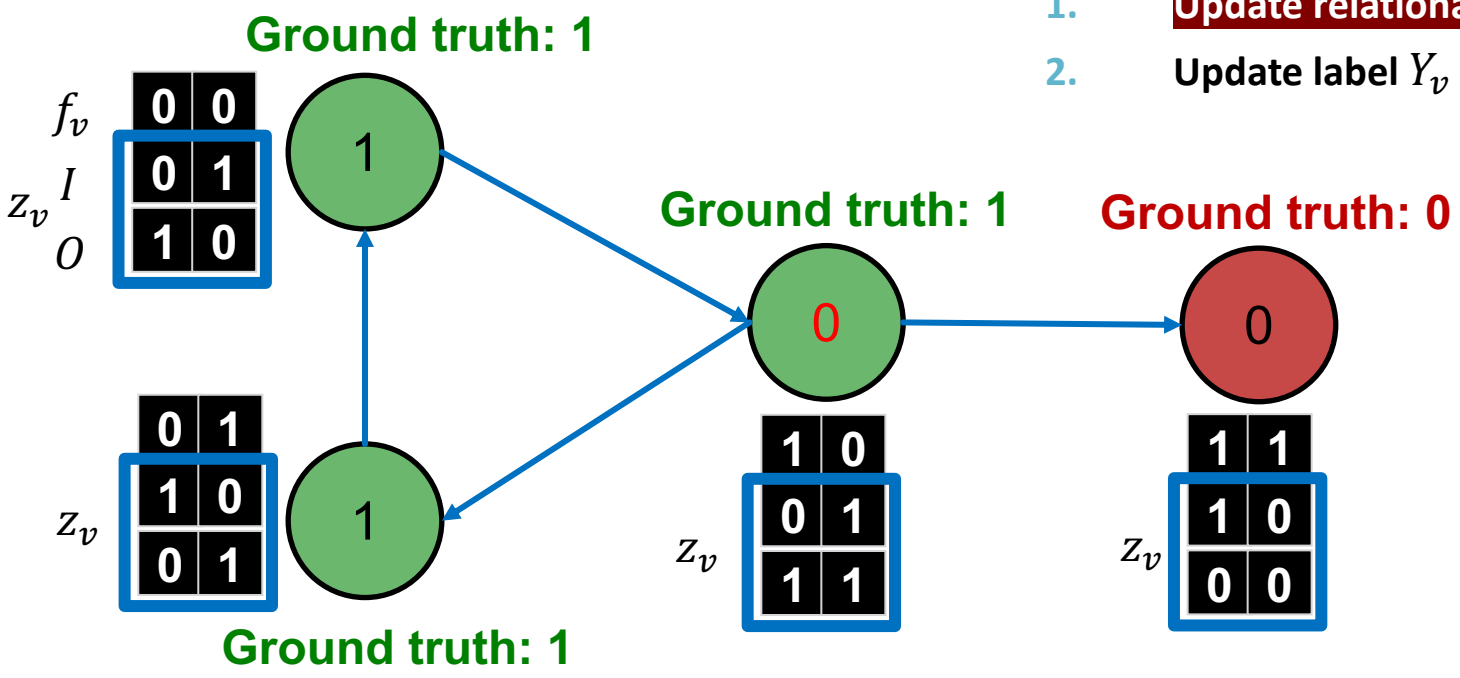
1. Train classifier
2. **Apply classifier to test set**
3. Iterate
   1. Update relational features z_v
   2. Update label Y_v



Iterative Classifier – Step 3.1

- Update z_v for all nodes

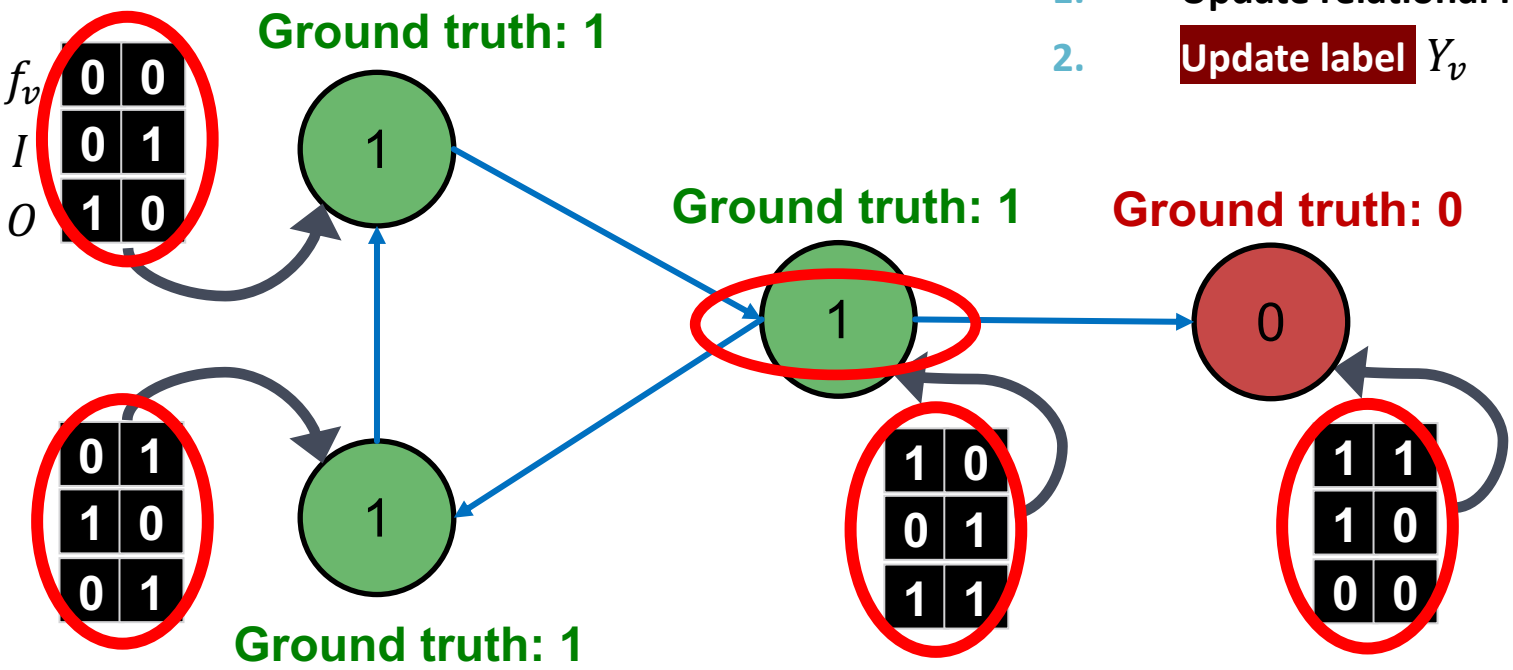
1. Train classifier
2. Apply classifier to test
3. Iterate
   1. Update relational features z_v
   2. Update label Y_v



Iterative Classifier – Step 3.2

- **Re-classify all nodes with ϕ_2**

1. Train classifier
2. Apply classifier to test
3. **Iterate**
   1. **Update relational features z_v**
   2. **Update label Y_v**

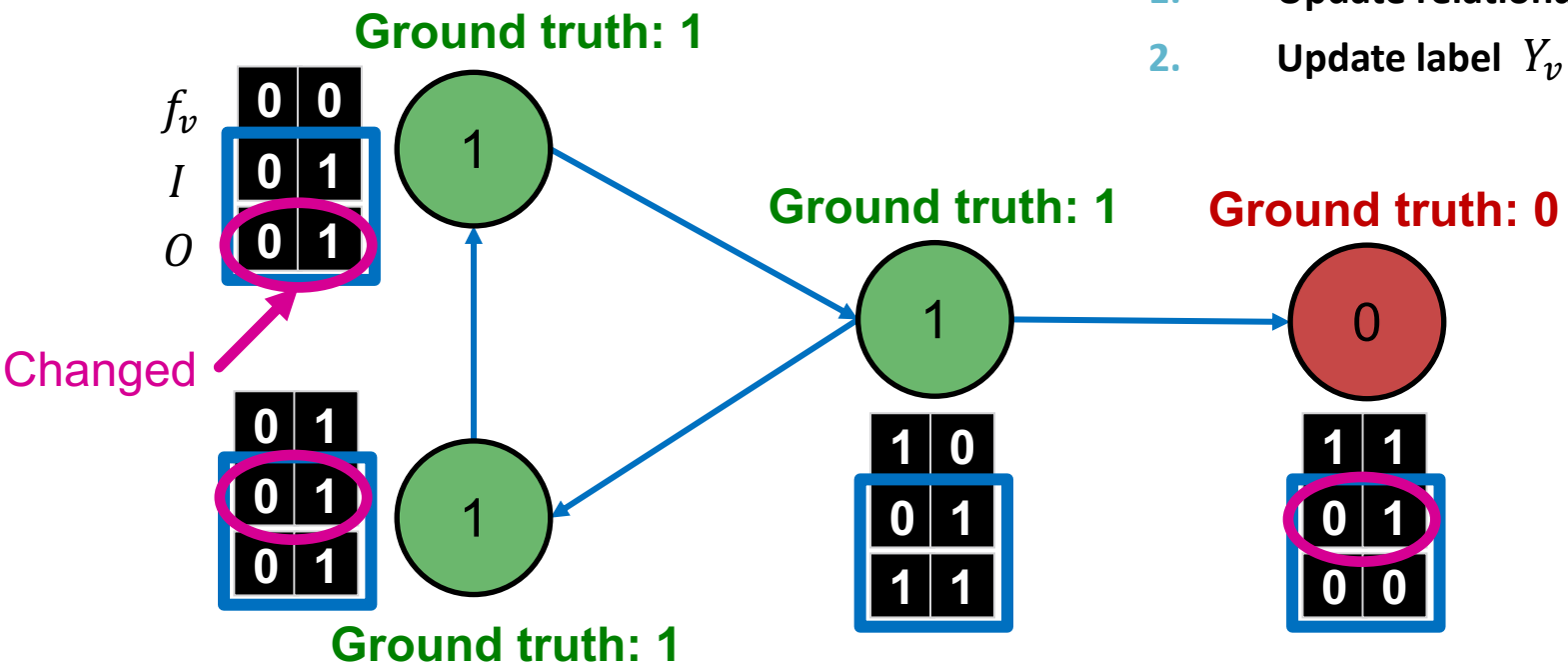


Now it's correct prediction!

Iterative Classifier – Iterate

- Continue until convergence
  - Update z_v
  - Update $Y_v = \phi_2(f_v, z_v)$

1. Train classifier
2. Apply classifier to test
3. **Iterate**
   1. Update relational features z_v
   2. Update label Y_v

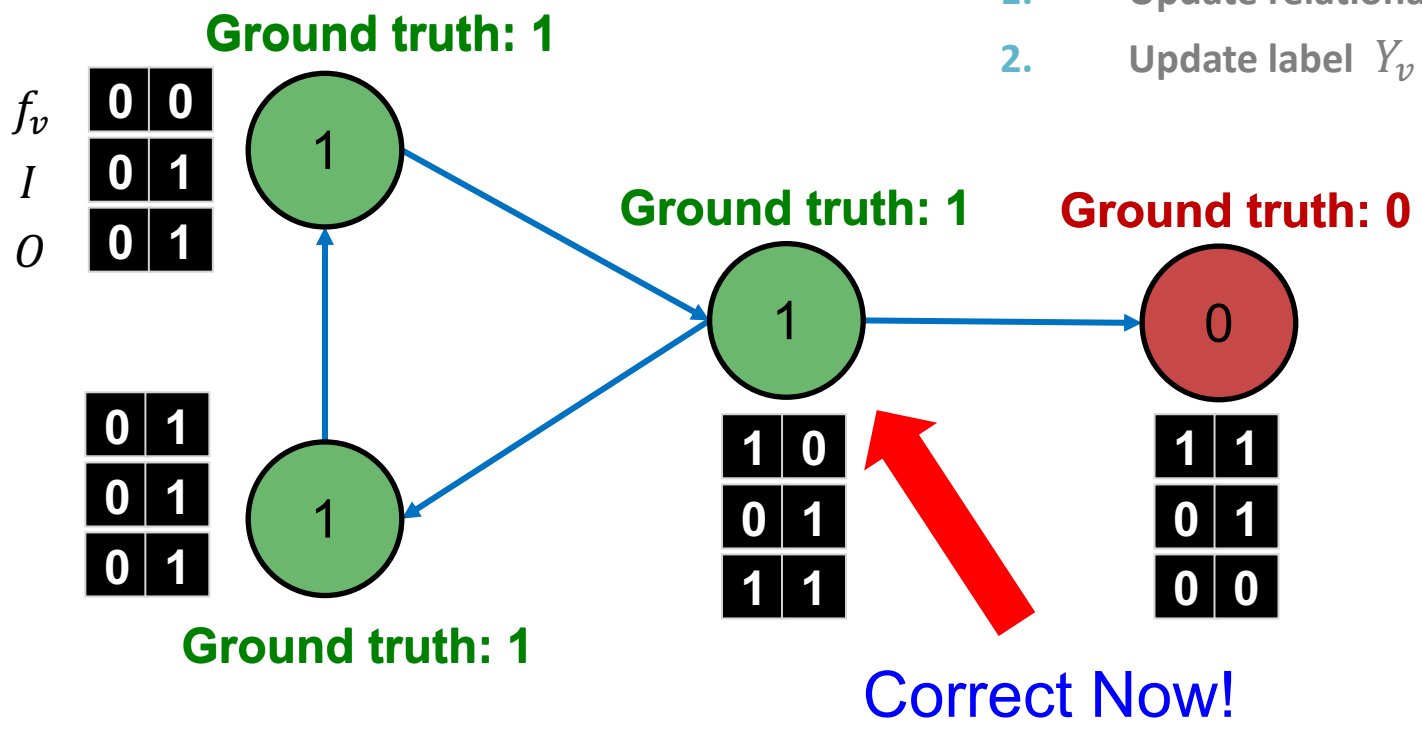


Iterative Classifier – Final Prediction

- Stop iteration
  - After convergence or when maximum iterations are reached

no labels change

1. Train classifier
2. Apply classifier to test set
3. Iterate
   1. Update relational features z_v
   2. Update label Y_v



Summary

- **We talked about 2 approaches to collective classification**
- **Relational classification** node labels + network structure; no node features
  - 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 i based on its **features** as well as **labels** of neighbors

$\phi_1(f_v) \rightarrow Y_v \rightarrow z_v \rightarrow \phi_2(f_v, z_v) \rightarrow$ Until Converges / Max iter.

Y_v: predicted; z_v: summary vector; ϕ_2: re-update

Stanford CS224W: Collective Classification: Belief Propagation

CS224W: Machine Learning with Graphs
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http://cs224w.stanford.edu

Collective Classification Models

- Relational classifiers
- Iterative classification
- **Loopy belief propagation**

Message Passing

Loopy Belief Propagation

- Belief Propagation is a dynamic programming approach to **answering probability queries in a graph** (e.g. probability of node v belonging to class 1)
- Iterative process in which neighbor nodes "talk" to each other, **passing messages**

"I (node v) believe you (node u) belong to class 1 with likelihood …"

- **When consensus is reached, calculate final belief**

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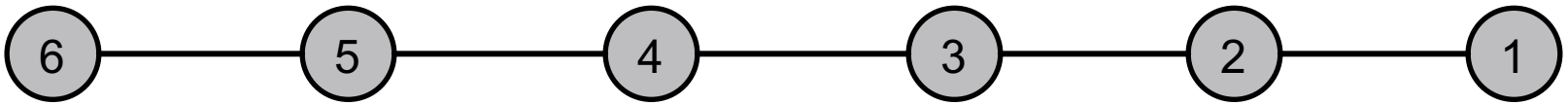
Message Passing: Basics

- **Task**: Count the number of nodes in a graph*
- **Condition:** Each node can only interact (pass message) with its neighbors

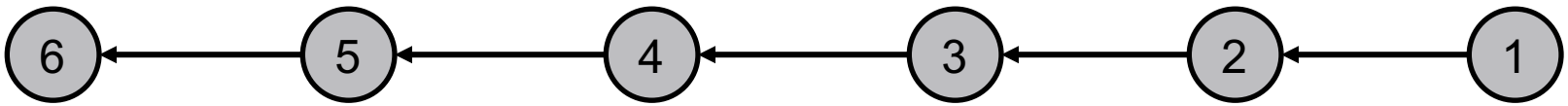
- **Example**: path graph



* Potential issues when the graph contains cycles.
We'll get back to it later!

Message Passing: Algorithm

- **Task**: Count the number of nodes in a graph
- **Algorithm**:
  - Define an ordering of nodes (that results in a path)
  - Edge directions are according to order of nodes
    - Edge direction defines the order of message passing
  - For node i from 1 to 6
    - Compute the message from node i to $i+1$ (number of nodes counted so far)
    - Pass the message from node i to $i+1$



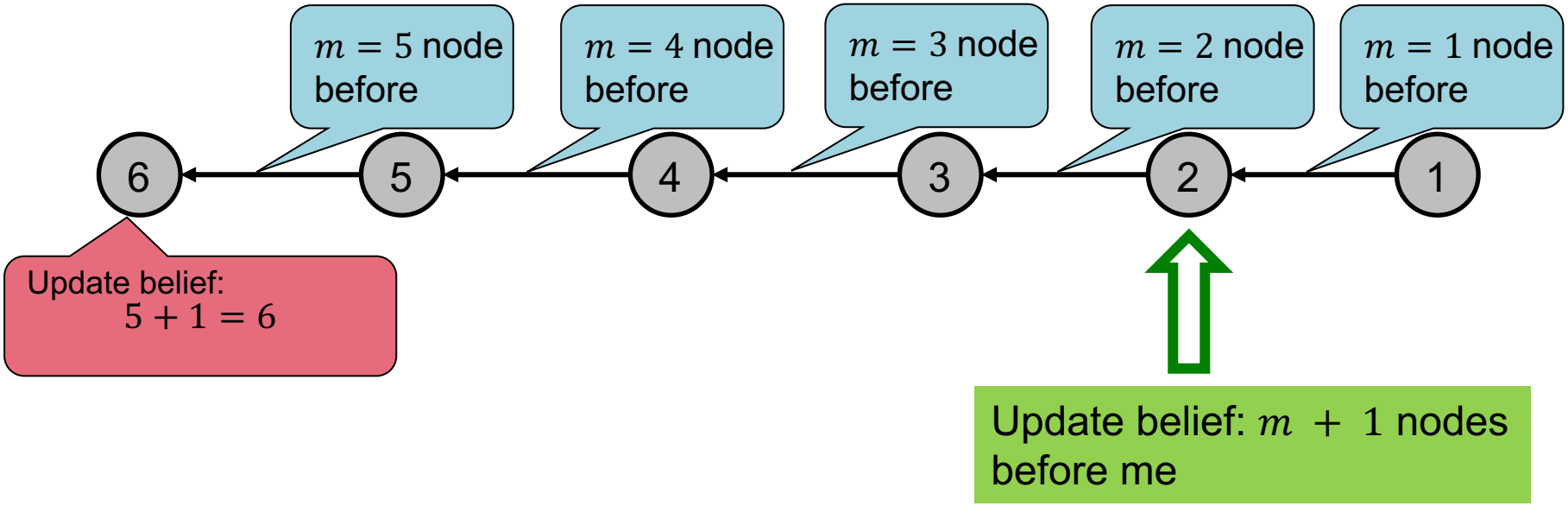
Message Passing: Basics

Task: Count the number of nodes in a graph

Condition: Each node can only interact (pass message) with its neighbors

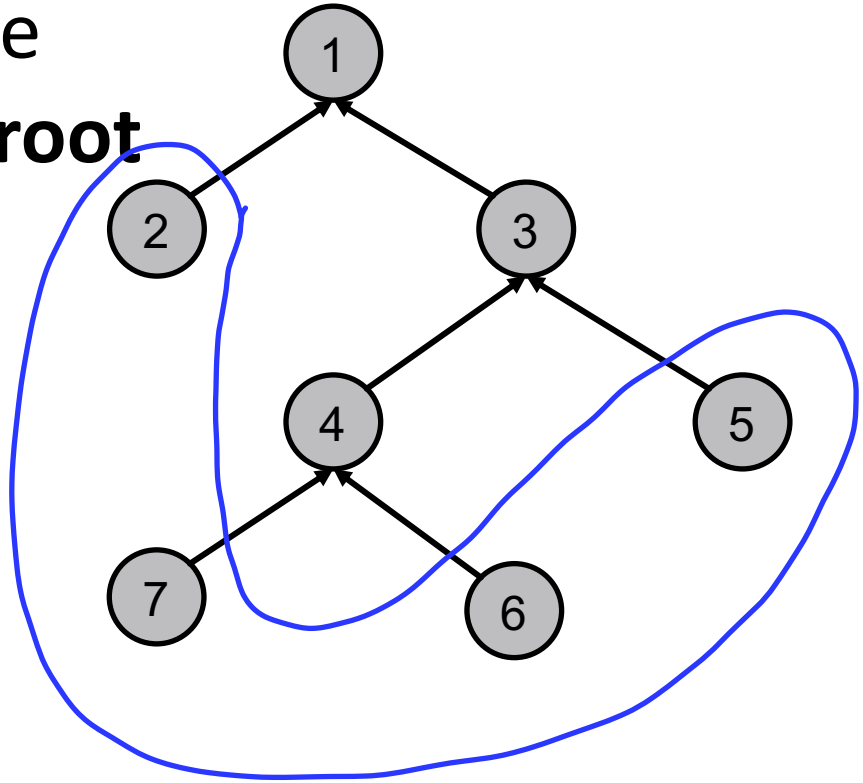
Solution: Each node listens to the message from its neighbor, updates it, and passes it forward

m: the message



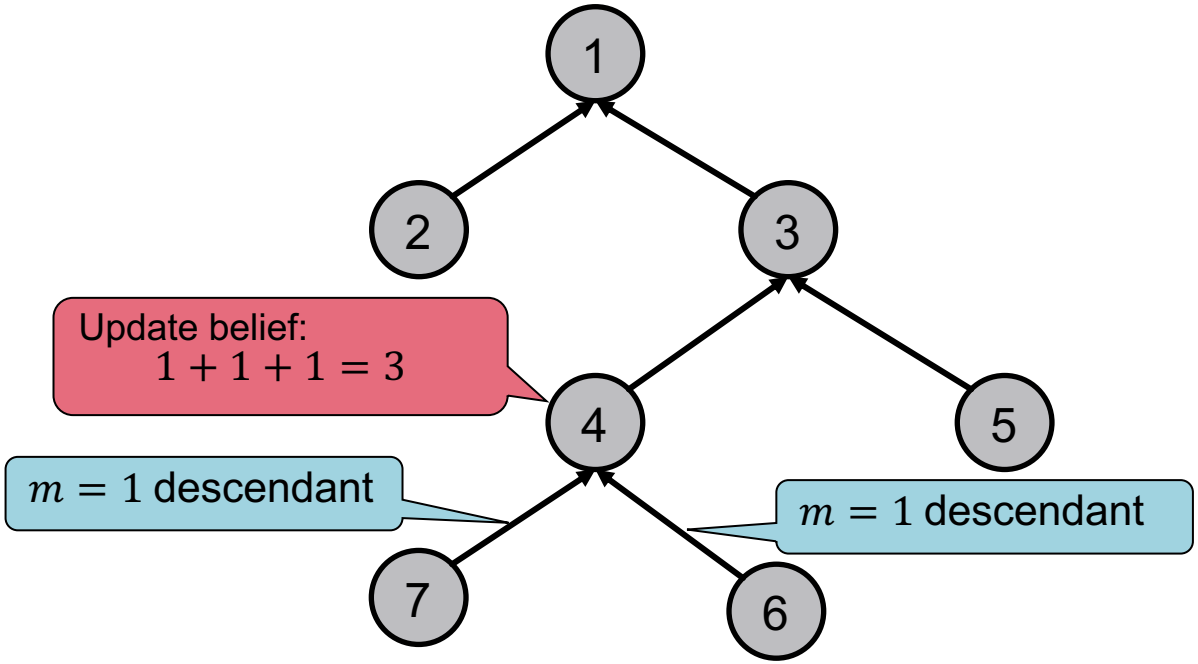
Generalizing to a Tree

- We can perform message passing not only on a path graph, but also on a tree-structured graph
- Define order of message passing from **leaves** to **root**



Message passing in a tree

Update beliefs in tree structure



Message passing in a tree

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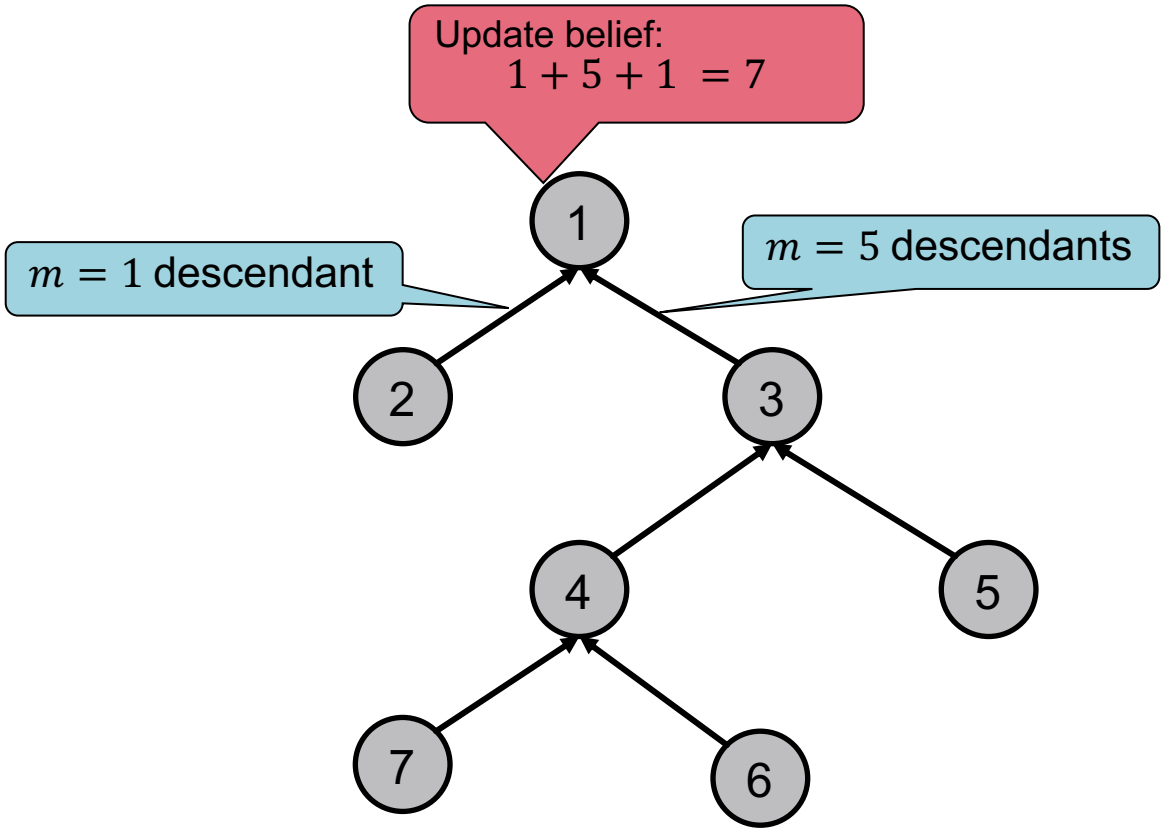
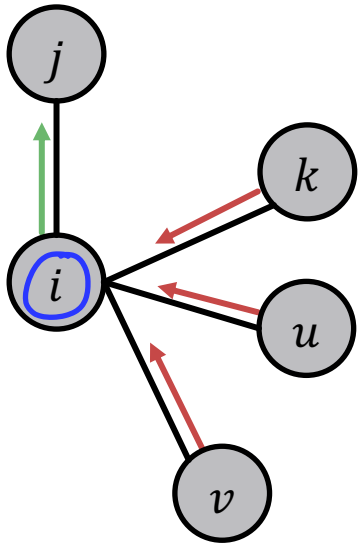


Loopy BP Algorithm



What message will i send to j?

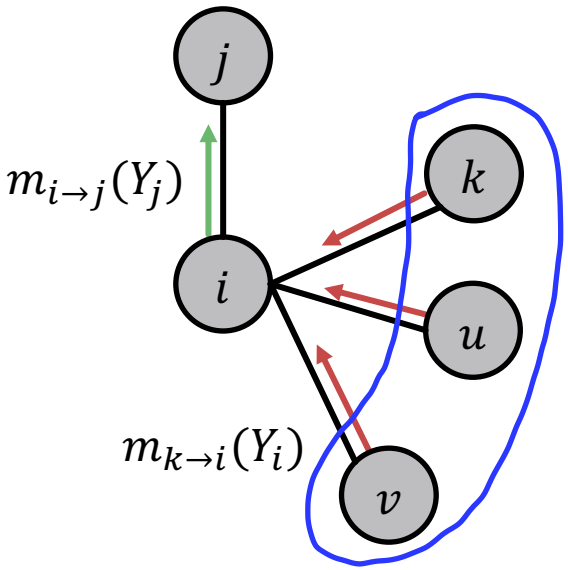
- It depends on what i hears from its neighbors
- Each neighbor passes a message to i its beliefs of the state of i

I (node i) believe that you (node j) belong to class Y_j with probability …

Notation

- ***Label-label potential matrix*** $\boldsymbol{\psi}$: Dependency between a node and its neighbor. $\boldsymbol{\psi}(Y_i, Y_j)$ is proportional to the probability of a node j being in class Y_j given that it has neighbor i in class Y_i. homophily
- ***Prior belief*** $\boldsymbol{\phi}$: $\phi(Y_i)$ is proportional to the probability of node i being in class Y_i.
- $m_{i \to j}(Y_j)$ is i's message / estimate of j being in class Y_j.
- $\mathcal{L}$ is the set of all classes/labels

Loopy BP Algorithm



1. Initialize all messages to 1
2. Repeat for each node:

how i's label should influence j's label

Label-label potential

All messages sent by neighbors from previous round

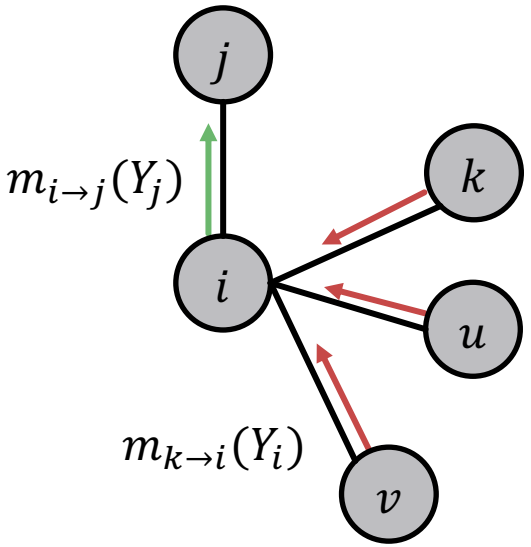
$$m_{i\to j}(Y_j) = \sum_{Y_i \in \mathcal{L}} \psi(Y_i, Y_j)\, \phi_i(Y_i) \prod_{k \in N_i \setminus j} m_{k\to i}(Y_i), \quad \forall Y_j \in \mathcal{L}$$

Sum over all states

Prior

omitting j

Loopy BP Algorithm



After convergence:

$b_i(Y_i)$ = node i's belief of being in class Y_i

All messages from neighbors

Prior

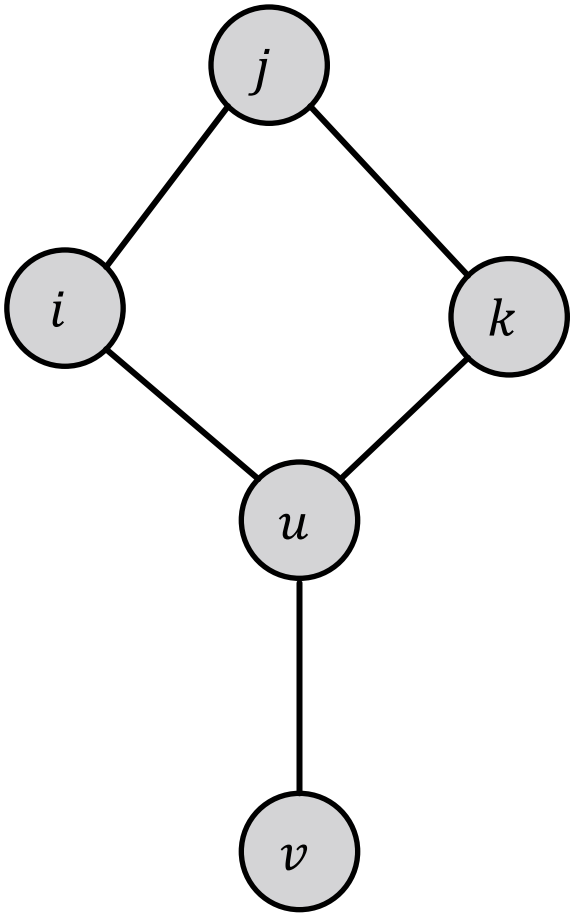
$$b_i(Y_i) = \phi_i(Y_i) \prod_{j \in N_i} m_{j\to i}(Y_i), \quad \forall\, Y_i \in \mathcal{L}$$

Example: Loopy Belief Propagation

- Now we consider a graph with cycles
- There is no longer an ordering of nodes
- We apply the same algorithm as in previous slides:
  - Start from arbitrary nodes
  - Follow the edges to update the neighboring nodes

Example: Loopy Belief Propagation

What if our graph has cycles?



Messages from different subgraphs are **no longer independent**!

But we can still run BP, but it will pass messages in loops.

Example: Loopy Belief Propagation

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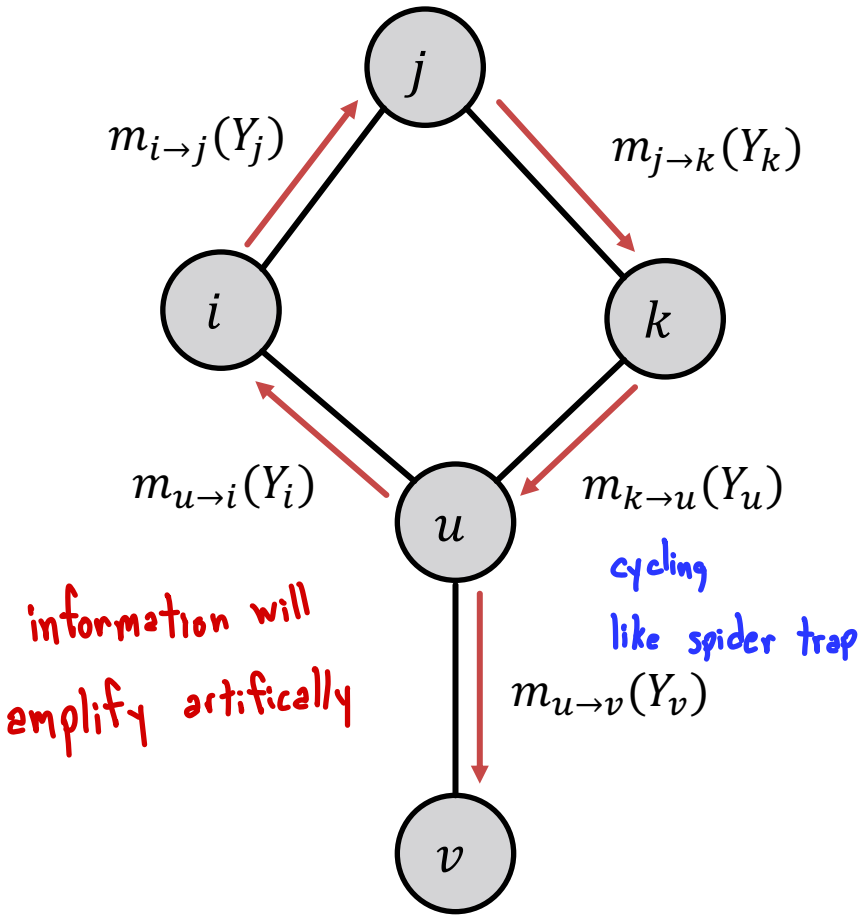

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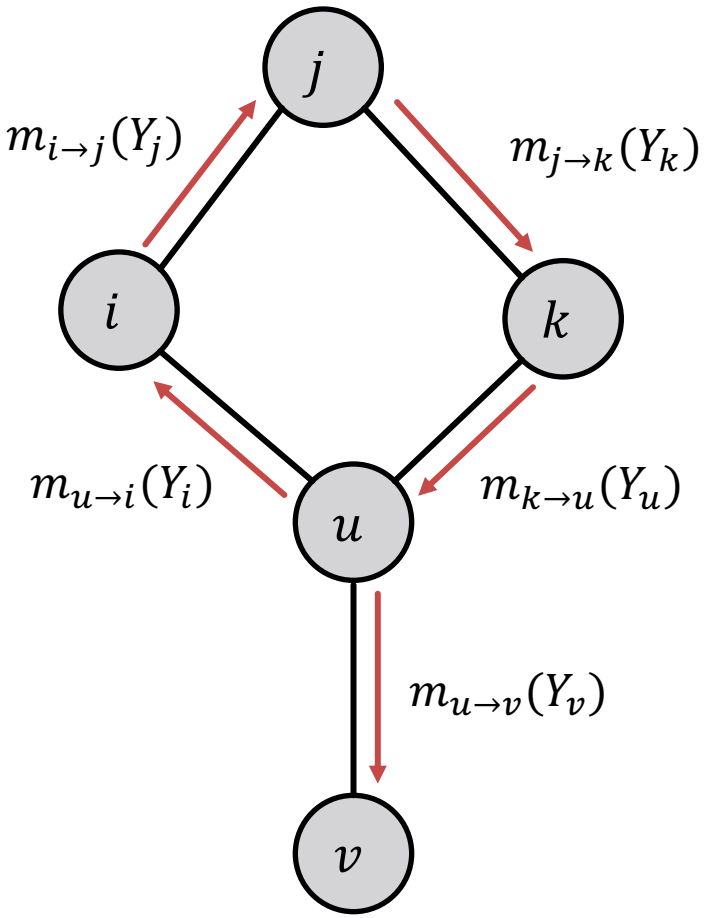
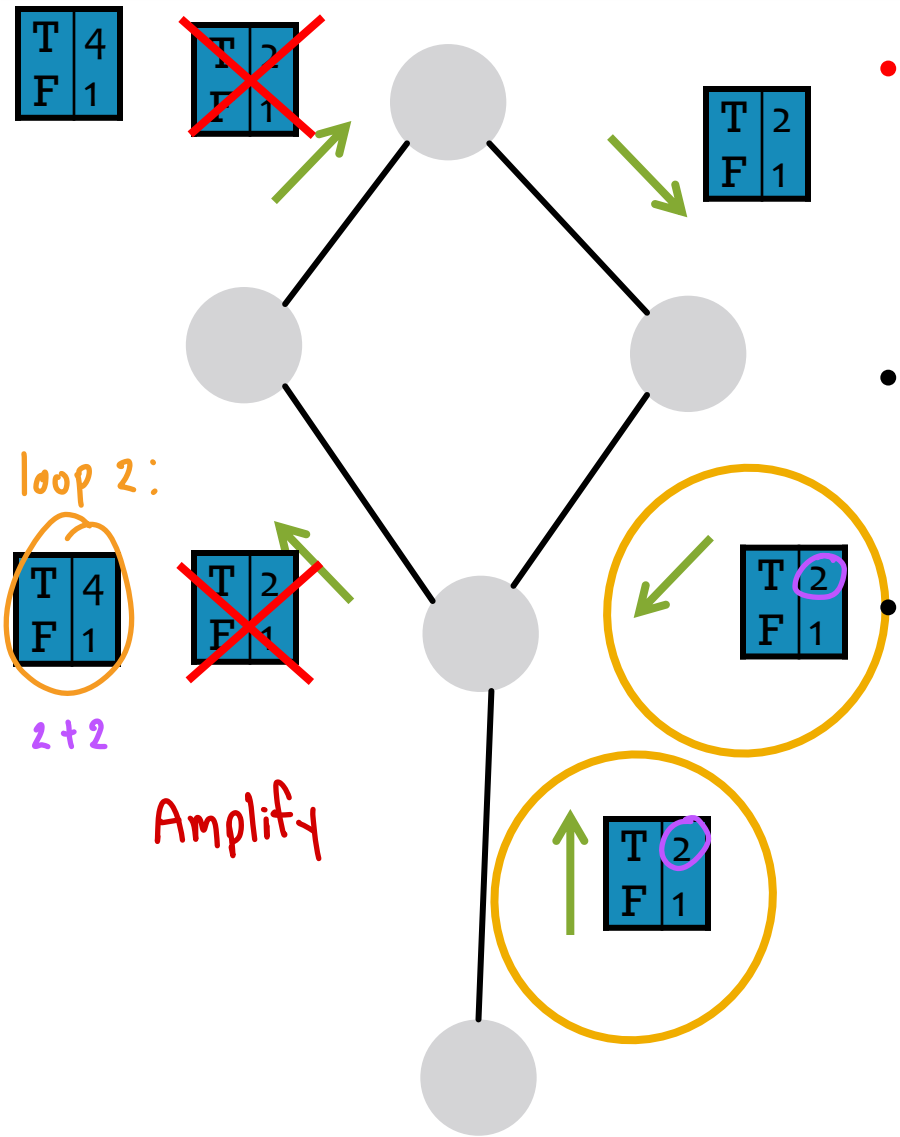
What Can Go Wrong?



- **Beliefs may not converge**
  - Message $m_{u\to i}(Y_i)$ is based on initial belief of i, not a **separate evidence** for i
  - The initial belief of i (which could be incorrect) is reinforced by the cycle $i \to j \to k \to u \to i$
- However, in practice, Loopy BP is still a good heuristic for complex graphs which contain many branches.

complex real-world nw tends to me more like trees. (small cycle)

What Can Go Wrong?



- Messages loop around and around: 2, 4, 8, 16, 32, ... More and more convinced that these variables are T!
- BP incorrectly treats this message as **separate evidence** that the variable is T (true).
- Multiplies these two messages as if they were independent.
  - But they don't actually come from *independent* parts of the graph.
  - One influenced the other (via a cycle).

This is an extreme example. Often in practice, the cyclic influences are weak. (As cycles are long or include at least one weak correlation.)

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Advantages of Belief Propagation

- **Advantages**:
  - Easy to program & parallelize
  - General: can apply to any graph model with any form of potentials
    - Potential can be higher order: e.g. $\boldsymbol{\psi}(Y_i, Y_j, Y_k, Y_v \ldots)$
- **Challenges**:
  - Convergence is not guaranteed (when to stop), especially if many closed loops tricks run BP for short ** steps
- **Potential functions** (parameters)
  - Require training to estimate label-label potential matrix ψ

Summary

- We learned how to leverage correlation in graphs to make prediction on nodes
- Key techniques:
  - Relational classification no features information
  - Iterative classification both node features + summary of the labels z_v
  - Loopy belief propagation label-label potential matrix ψ
    - collecting messages → send to the upstream neighbor
    - well-defined on chain graphs & trees
    - problem on graph with cycles, in practice cycles don't cause too much problem.
    - BP strong for semi-supervised labelling of nodes in the graph