Stanford CS224W: Label Propagation on Graphs

CS224W: Machine Learning with Graphs

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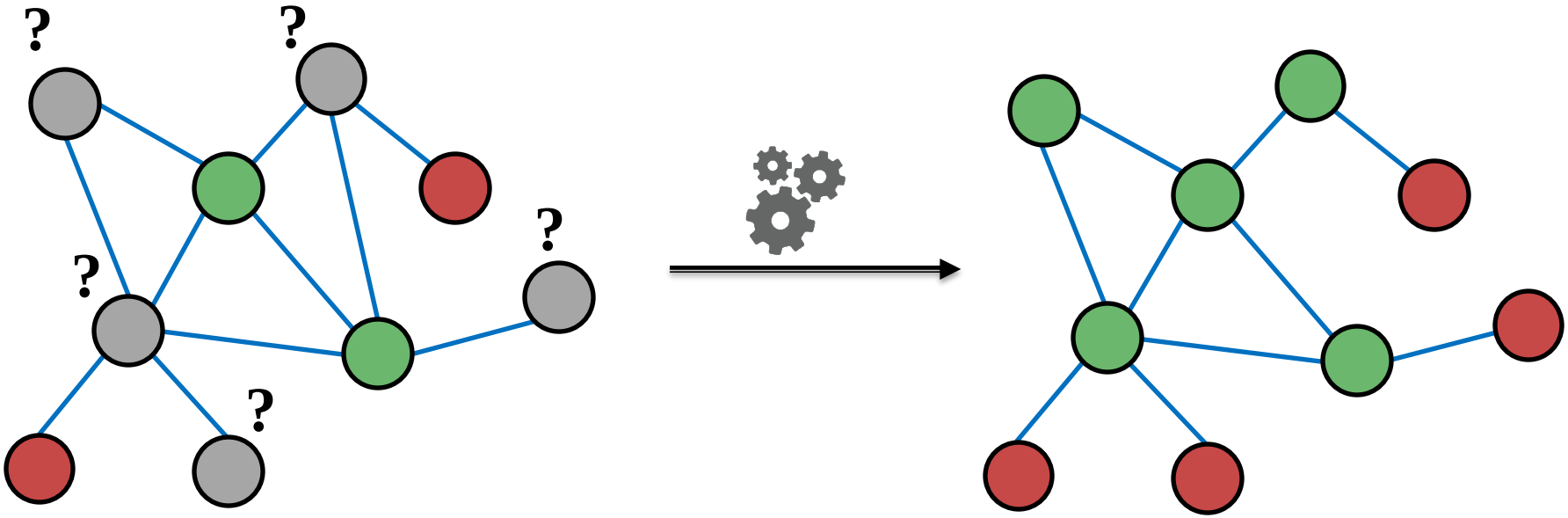
http://cs224w.stanford.edu

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?**
- **Node embeddings** (from **random walks, GNN**) is a method to solve this problem
  - Are there alternative solutions based on the network topology?

Setting: Node Classification



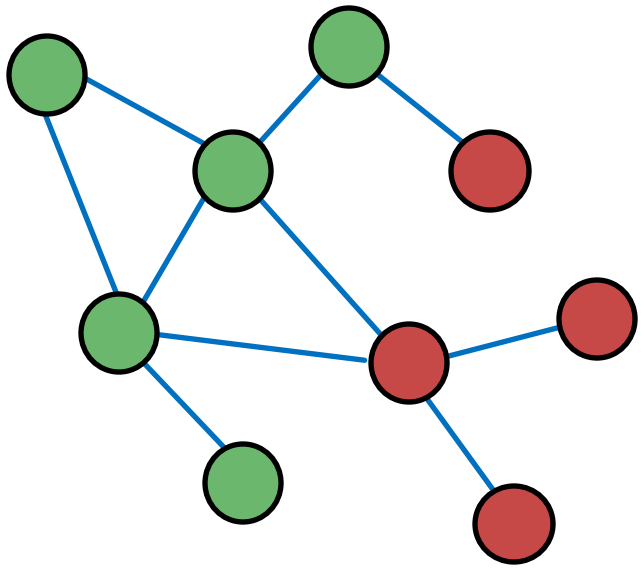
- Given labels of some nodes
- Let's predict labels of unlabeled nodes
- **Transductive node classification** (also called **semi-supervised node classification**)

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: Label propagation**
- **Intuition: Correlations** exist in networks.
  - Connected nodes tend to share the same label
- **We will look at three techniques today:**
  - **Label propagation**
  - **Correct & Smooth**
  - **Masked label prediction**

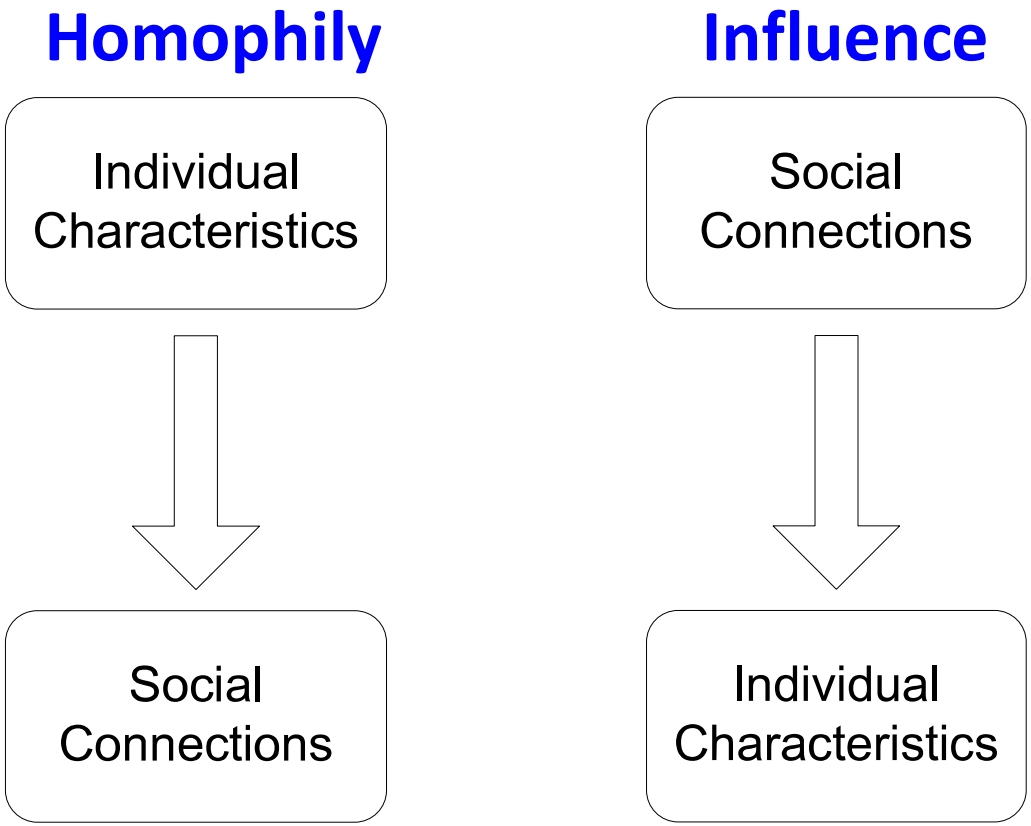
Observation: Correlations in Networks

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



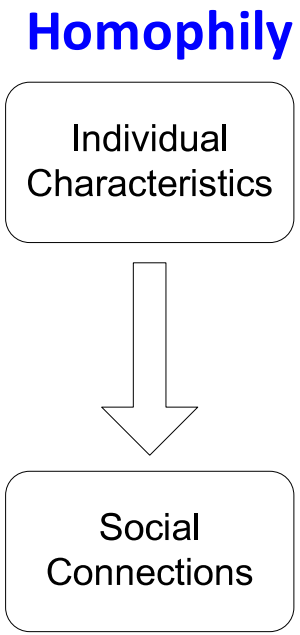
Correlations Exist in Networks

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



Social Homophily

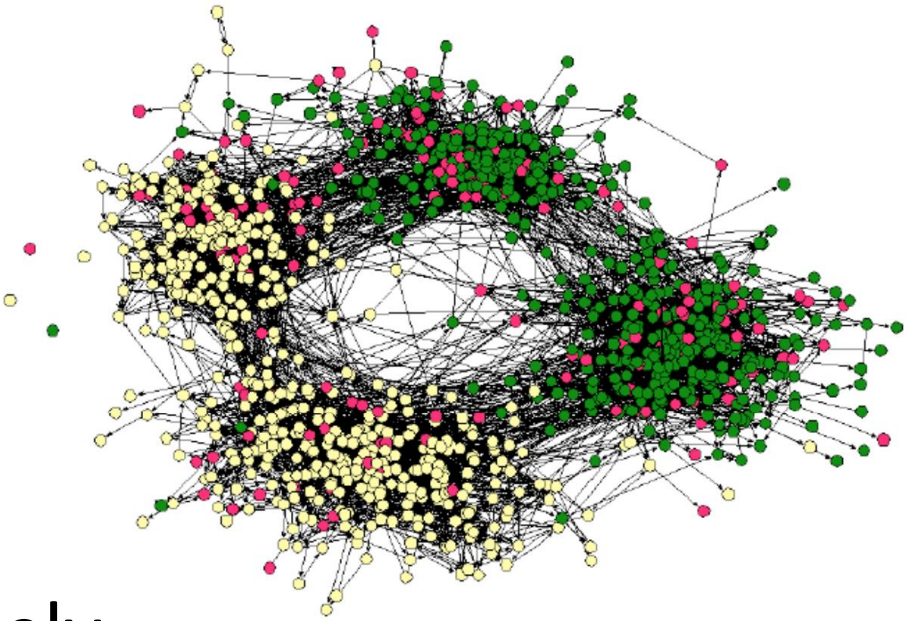
- **Homophily**: The tendency of individuals to associate and bond with similar others
  - *"Birds of a feather flock together"*
  - It has been observed in a vast array of network studies, based on a variety of attributes (e.g., age, gender, organizational role, etc.)
  - **Example**: Researchers who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



Homophily: Example

Example of homophily

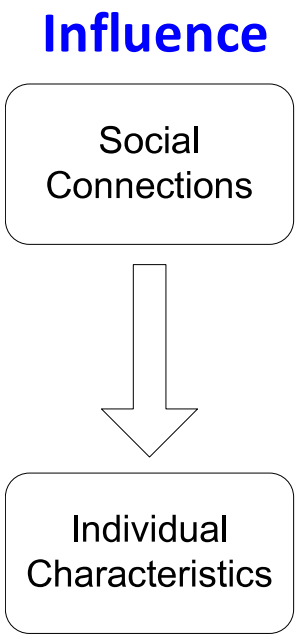
- Online social network
  - Nodes = people
  - Edges = friendship
  - Node color = interests (sports, arts, etc.)
- People with the same interest are more closely connected due to homophily



(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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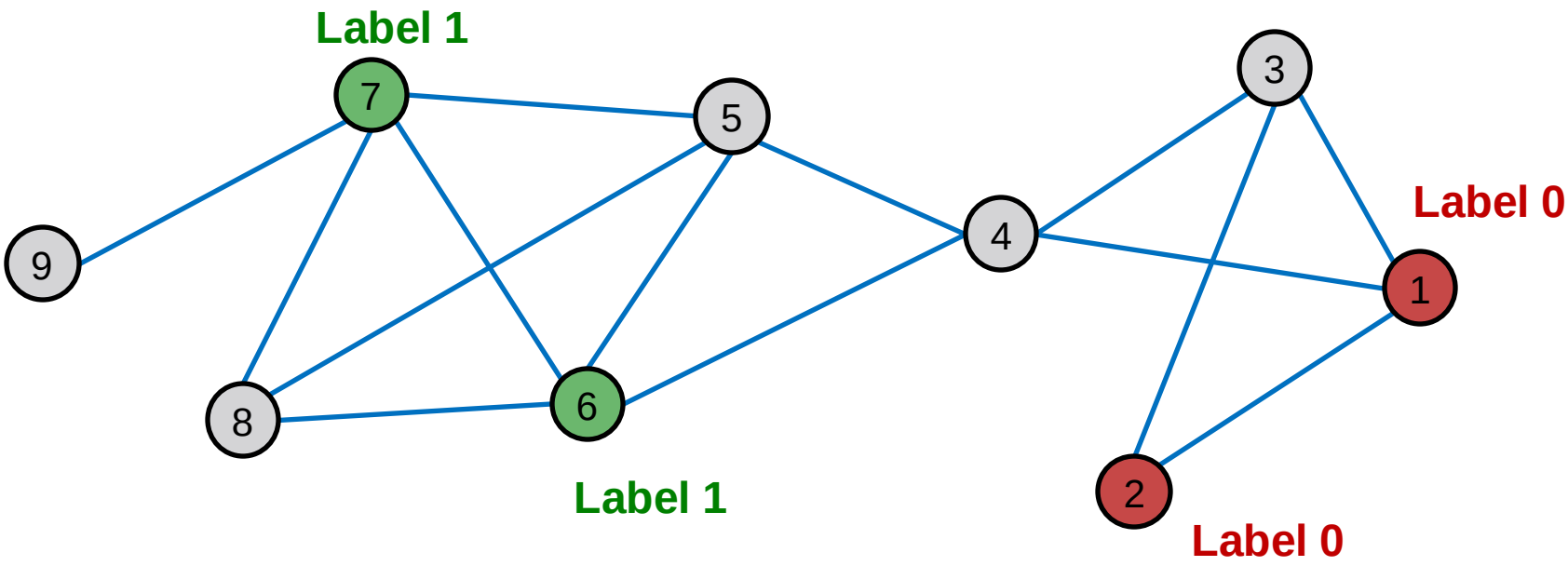
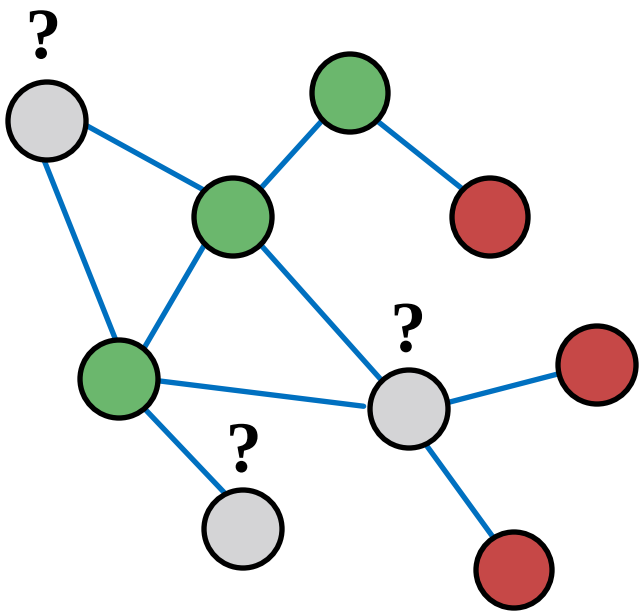
Classification with Network Data

- **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?

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)

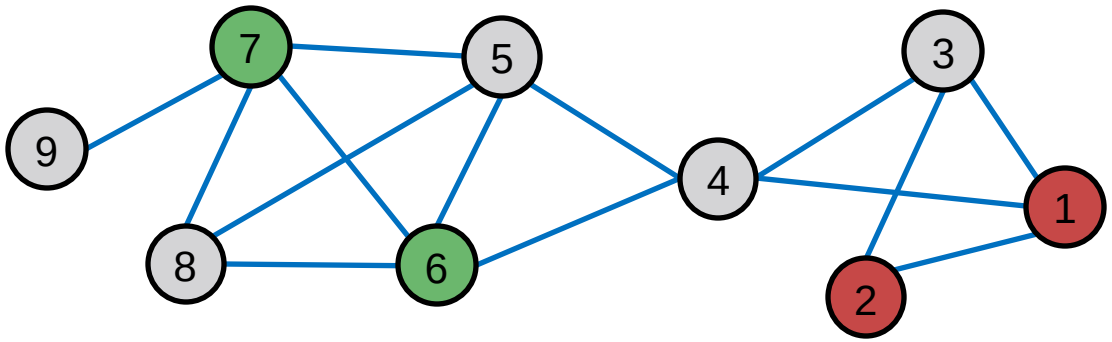
Example task:

- Let $\boldsymbol{A}$ 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**

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

- We focus on **semi-supervised binary node classification**
- **We will introduce three approaches:**
  - **Label propagation**
  - **Correct & Smooth**
  - **Masked label prediction**

Stanford CS224W: Label Propagation

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Label Propagation (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 unlabeled nodes** (in parallel or a random order) until convergence or until maximum number of iterations is reached.

Label Propagation (2)

- **The math: Update each unlabeled node** v label

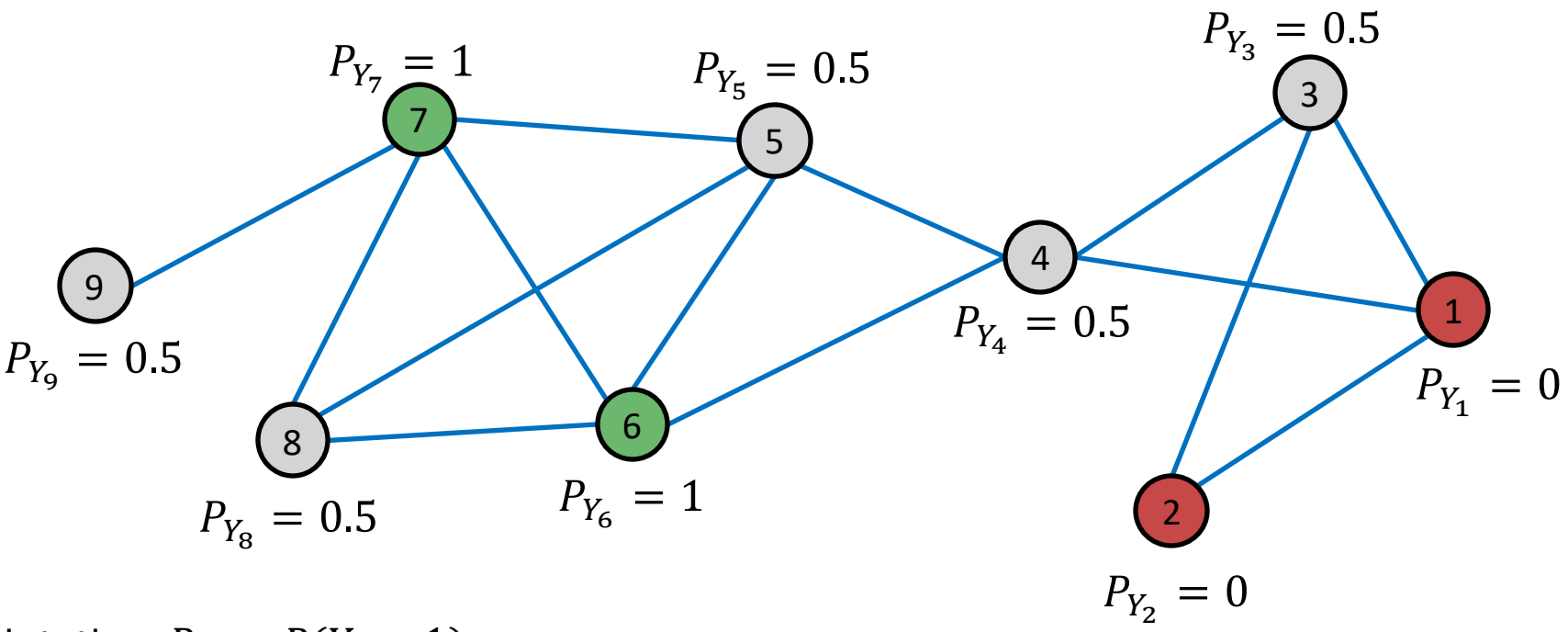
$$P^{(t+1)}(Y_v = c) = \frac{1}{\sum_{(v,u)\in E} A_{v,u}} \sum_{(v,u)\in E} A_{v,u}\, P^{(t)}(Y_u = c)$$

  - 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.
  - **Repeated** the update until convergence

Example: Initialization

Initialization:

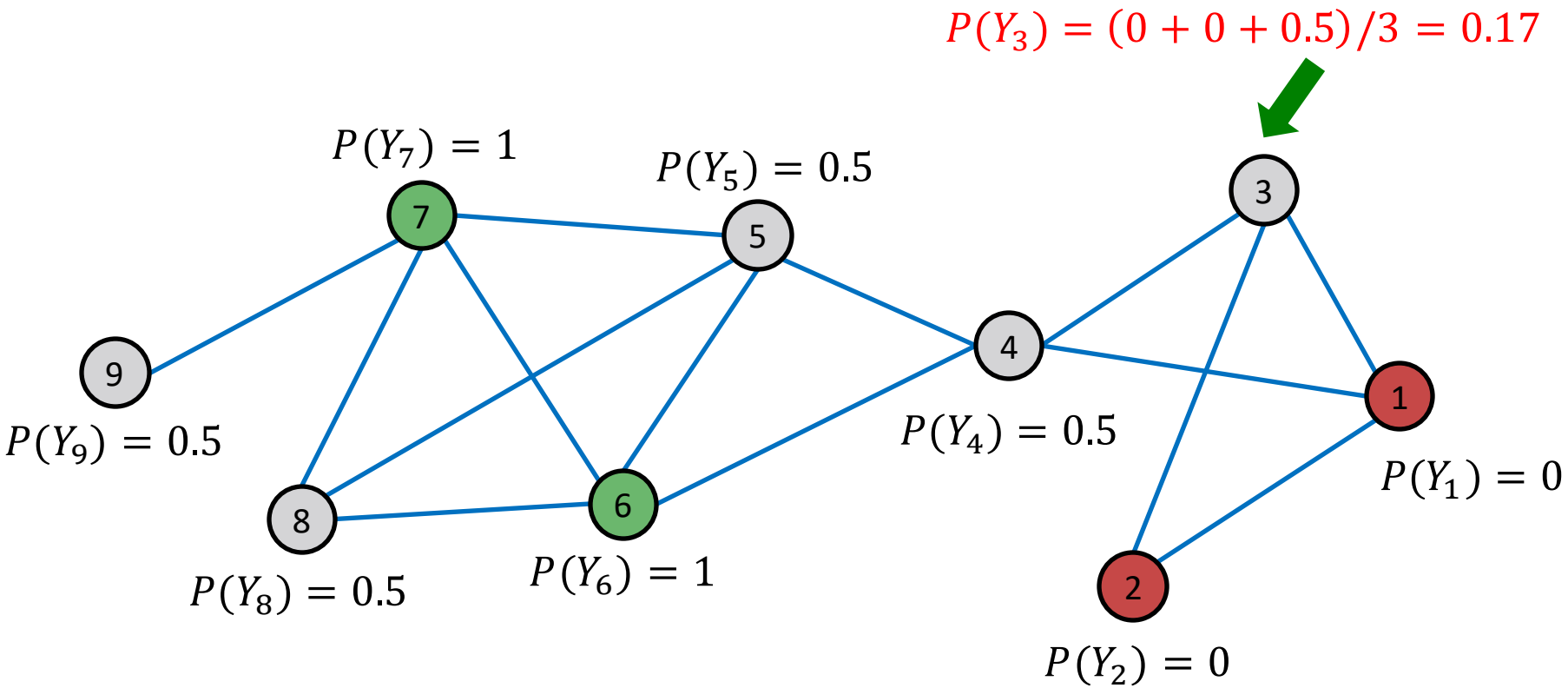
- All labeled nodes with their labels
- All unlabeled nodes 0.5 (belonging to class 1 with probability 0.5)



Notation: $P_{Y_1} = P(Y_1 = 1)$

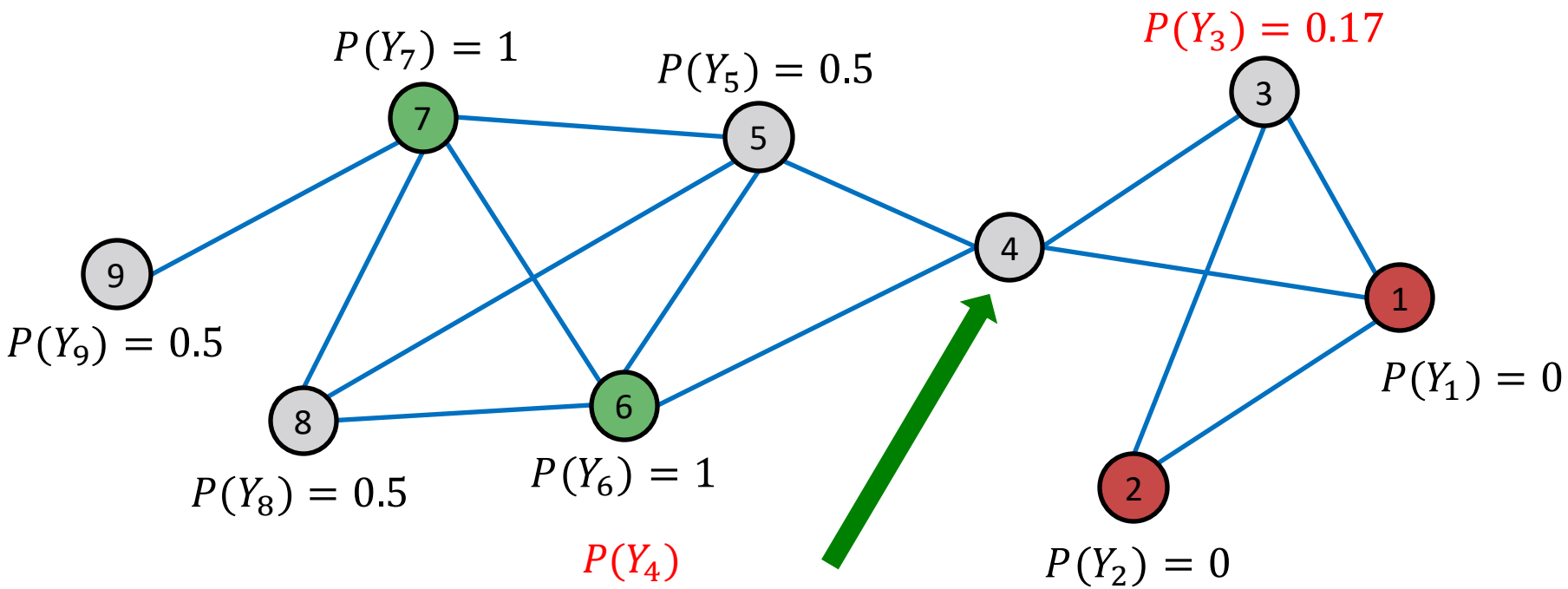
Example: 1st Iteration, Update Node 3

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



Example: 1st Iteration, Update Node 4

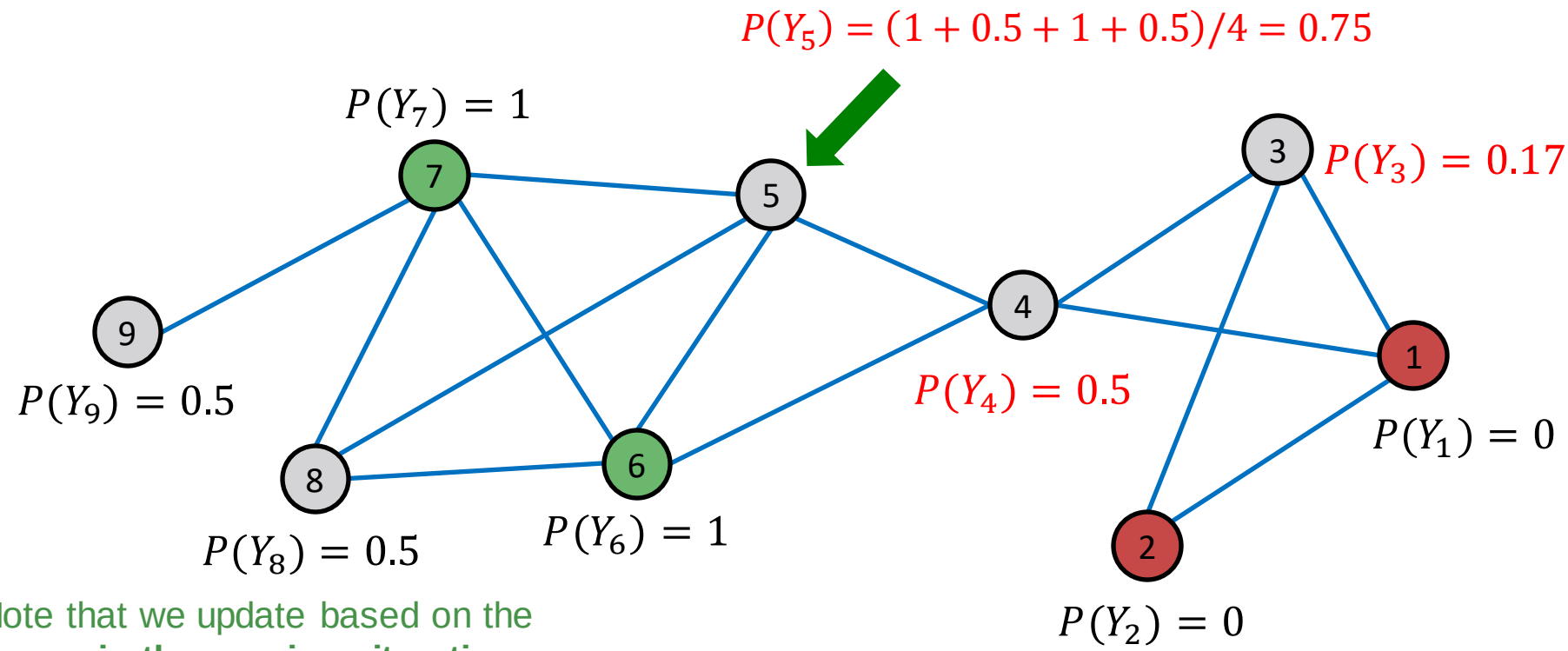
- Update for the 1st Iteration:
  - For node 4, $N_4 = \{1, 3, 5, 6\}$



Note that we update based on the scores **in the previous iteration**

Example: 1st Iteration, Update Node 5

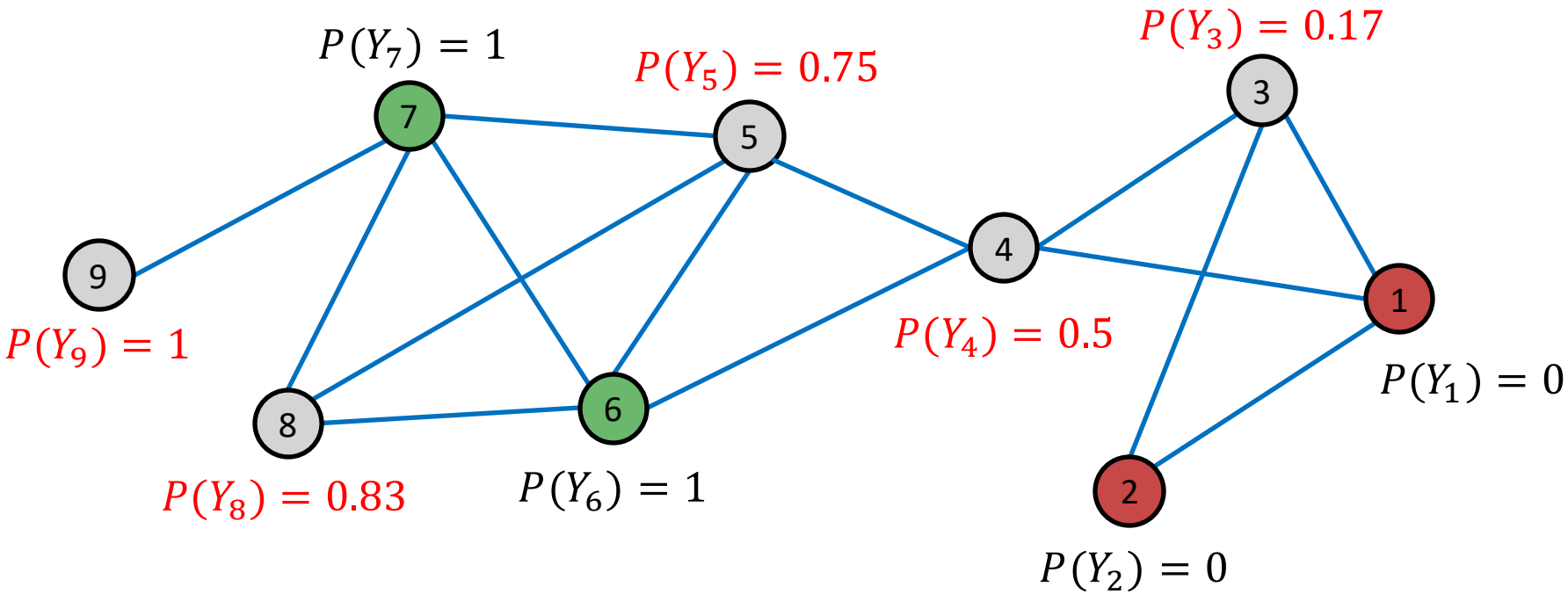
- Update for the 1st Iteration:
  - For node 5, $N_5 = \{4, 6, 7, 8\}$



Note that we update based on the scores **in the previous iteration**

Example: After 1st Iteration

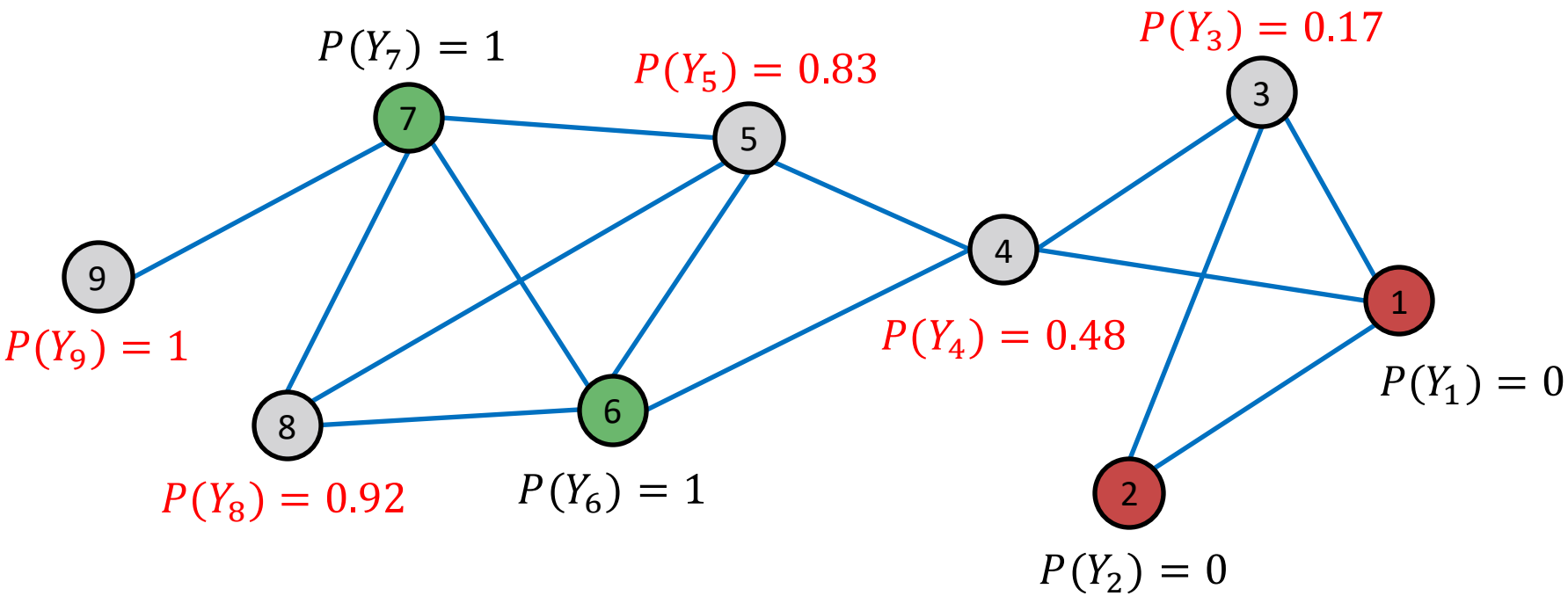
After Iteration 1 (a round of updates for all unlabeled nodes)



Note that we update based on the scores **in the previous iteration**

Example: After 2nd Iteration

After Iteration 2



Label Propagation: Convergence

- Intuition: Stop iterating when all nodes have reached a static value. Applying label propagation does not change labels anymore.
- **Convergence criteria:**

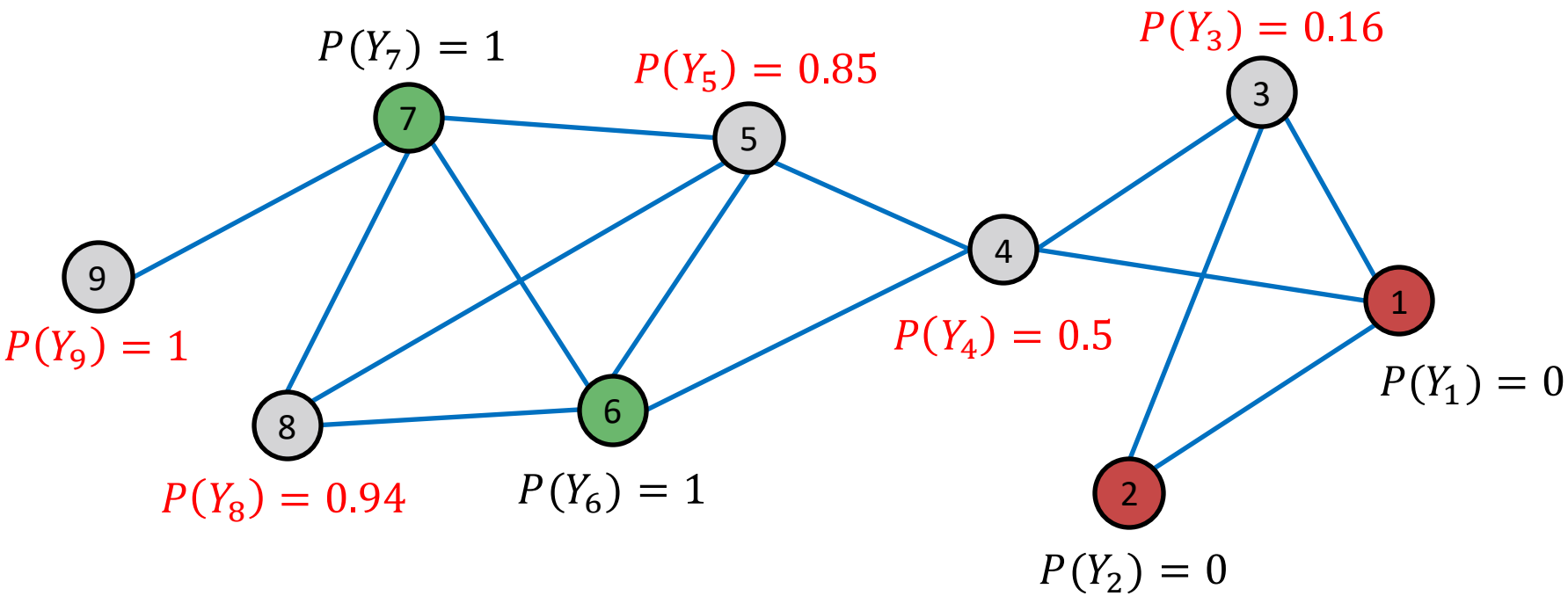
$$\left| P^{(t)}(Y_v) - P^{(t-1)}(Y_v) \right| \leq \epsilon$$

for all nodes v.

Here ϵ is the convergence threshold.

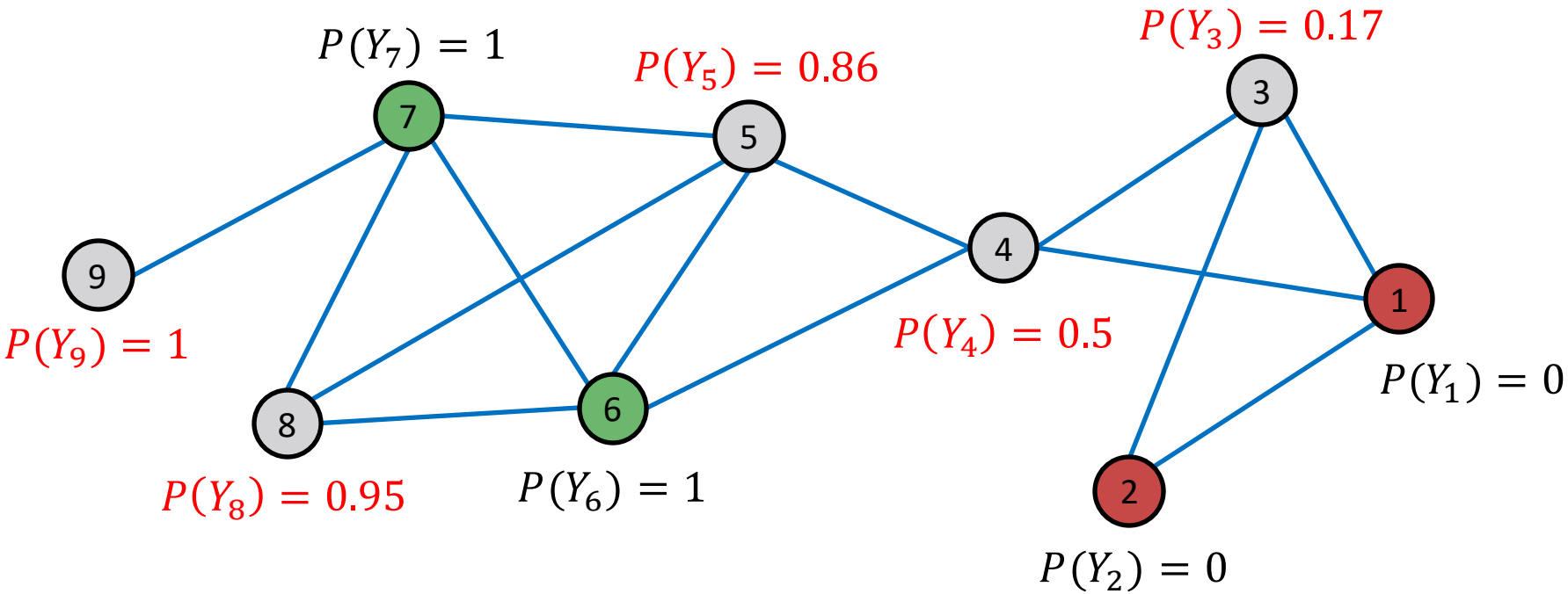
Example: After 3rd Iteration

After Iteration 3



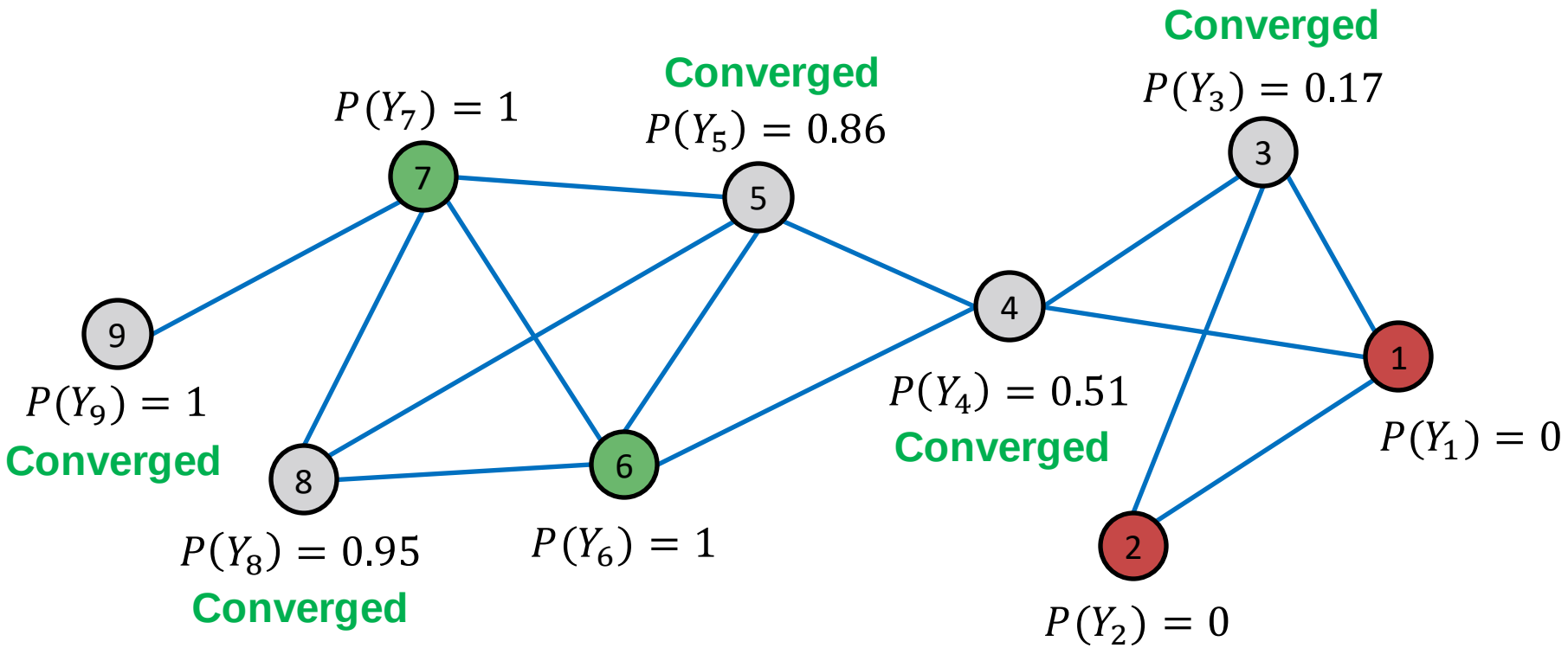
Example: After 4th Iteration

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** ($P_{Y_v} < 0.5$)



Label Propagation Applications

- **Document classification**
  - Nodes: documents
  - Edges: document similarity (e.g. word overlap)
- **Twitter polarity classification**
  - Nodes: users, tweets, words, hashtags, emoji
  - Edges [users -> users] Twitter follower graph;
    Edges [users -> tweets] creation;
    Edges [tweets -> words/hashtags/emoji] part of.
- **Spam and fraud detection**

Summary

- **Label propagation**
  - Iteratively update probabilities of node belonging to a label class based on its neighbors
- **Issue**
  - Convergence may be **very slow** and not **guaranteed**
  - **Label propagation does not use node attributes**
  - Can we improve the idea of label propagation to **leverage attribute/feature information?**

Stanford CS224W: Node Classification: Correct & Smooth

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Correct & Smooth

[Huang et al., ICLR 2021]

- **Correct & Smooth (C&S), recent state-of-the-art node classification method.**

Leaderboard for ogbn-products

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

Package: >=1.1.1

Rank	Method	Ext. data	Test Accuracy	Validation Accuracy	Contact	References	#Params	Hardware	Date
1	GLEM+EnGCN	Yes	0.9014 ± 0.0012	0.9370 ± 0.0004	Jianan Zhao (Mila & MSRA Team)	Paper, Code	139,633,805	Tesla V100 (32GB)	Oct 27, 2022
2	EnGCN	No	0.8798 ± 0.0004	0.9241 ± 0.0003	Keyu Duan (NUS)	Paper, Code	653,918	GeForce RTX 3090 (24GB)	Oct 23, 2022
3	GLEM+GIANT+SAGN+SCR	Yes	0.8737 ± 0.0006	0.9400 ± 0.0003	Jianan Zhao (Mila & MSRA Team)	Paper, Code	139,792,525	Tesla V100 (32GB)	Oct 27, 2022
4	GIANT-XRT+R-SAGN+SCR+C&S	Yes	0.8684 ± 0.0005	0.9365 ± 0.0003	LeeXue (HIT Team)	Paper, Code	1,154,142	TITAN RTX (24GB GPU)	Sep 30, 2022

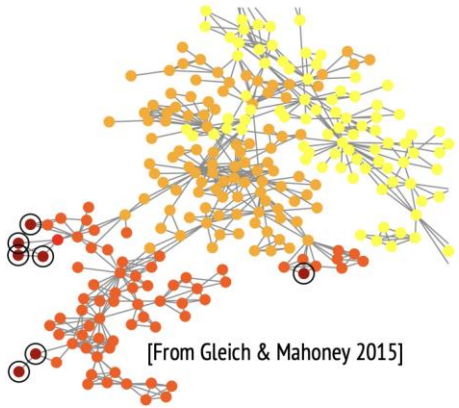
C&S tops the OGB leaderboard!

OGB leaderboard snapshot at Jan 30, 2023

[Adapted from "Label Propagation and Graph Neural Networks"]

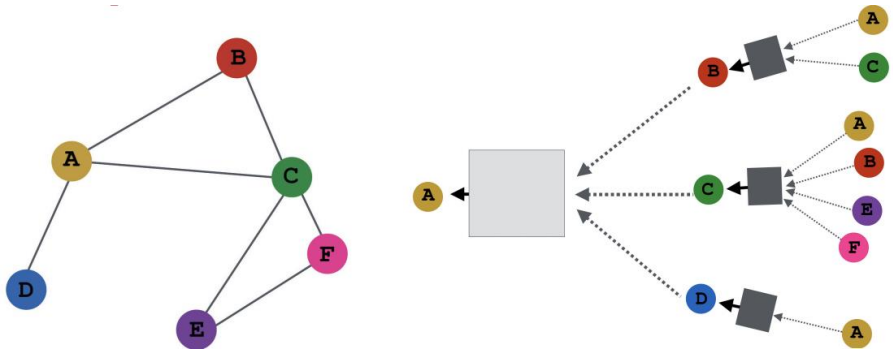
Correct & Smooth: Motivations

Label Propagation (LP)



- Modeling assumption: connected nodes have similar labels.
- Works because of homophily a.k.a. associativity
- **FAST**: few sparse matrix-vector products
- **Why not use additional info or features?**

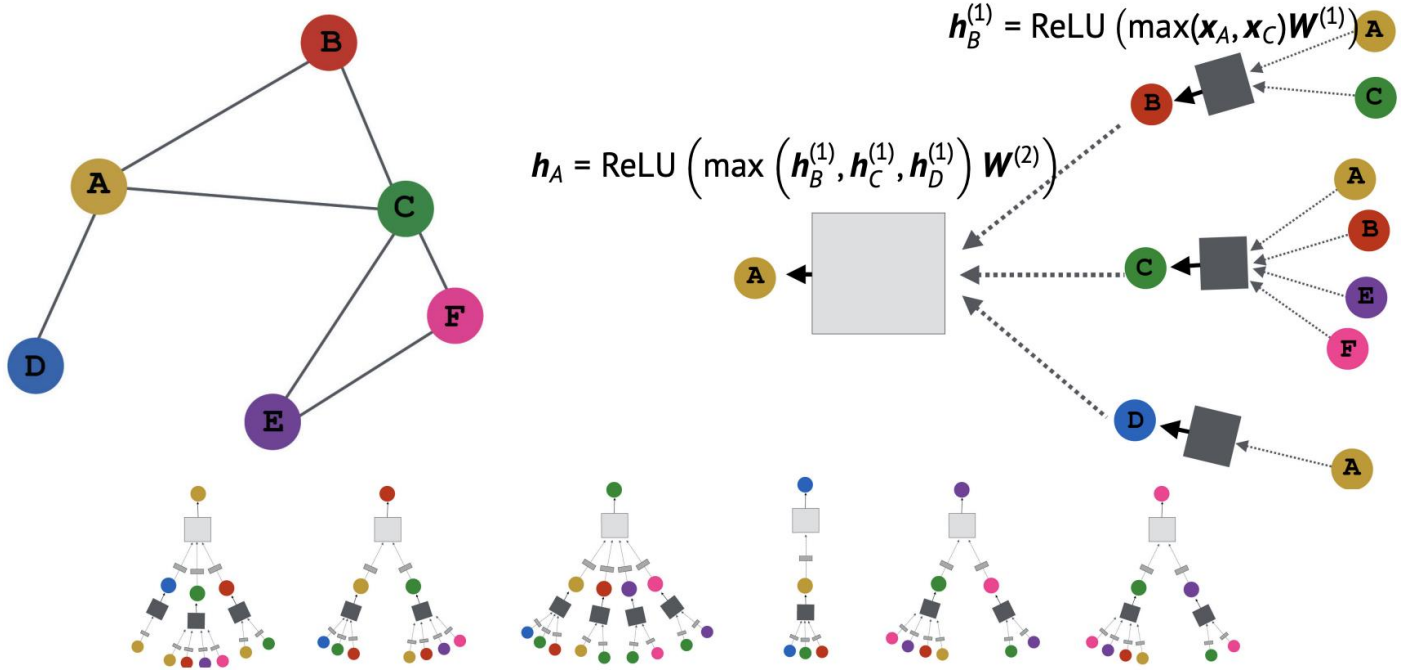
Graph Neural Networks



- Modeling assumption: labels only depend on neighbor features.
- Works because these features are sometimes very informative.
- **SLOW**: many parameters, irregular computation
- **Why not assume labels are correlated?**

[Adapted from "Label Propagation and Graph Neural Networks"]

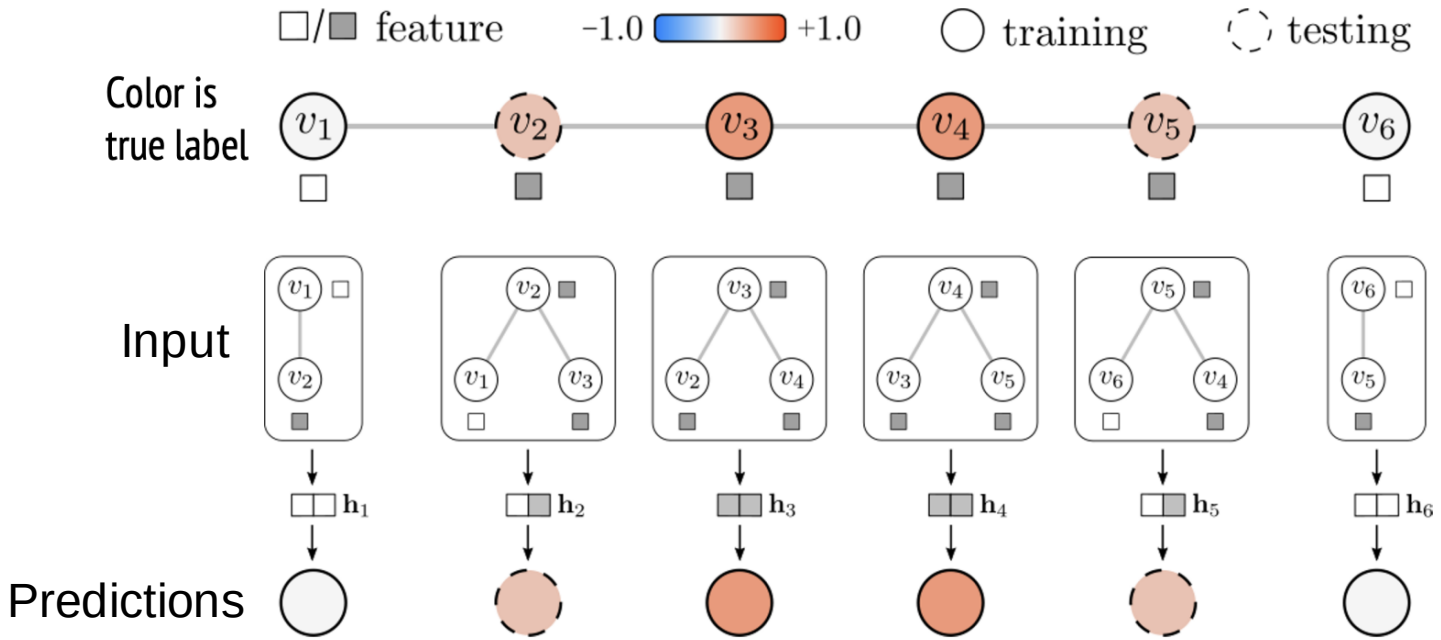
GNNs make uncorrelated predictions



- **GNN uses labels to train the weights** of a model
  - Given a trained model, **predictions for different node are independent/uncorrelated**.
- In contrast, **LP directly uses the labels in predictions.**

[Adapted from "Label Propagation and Graph Neural Networks"]

GNNs make uncorrelated predictions



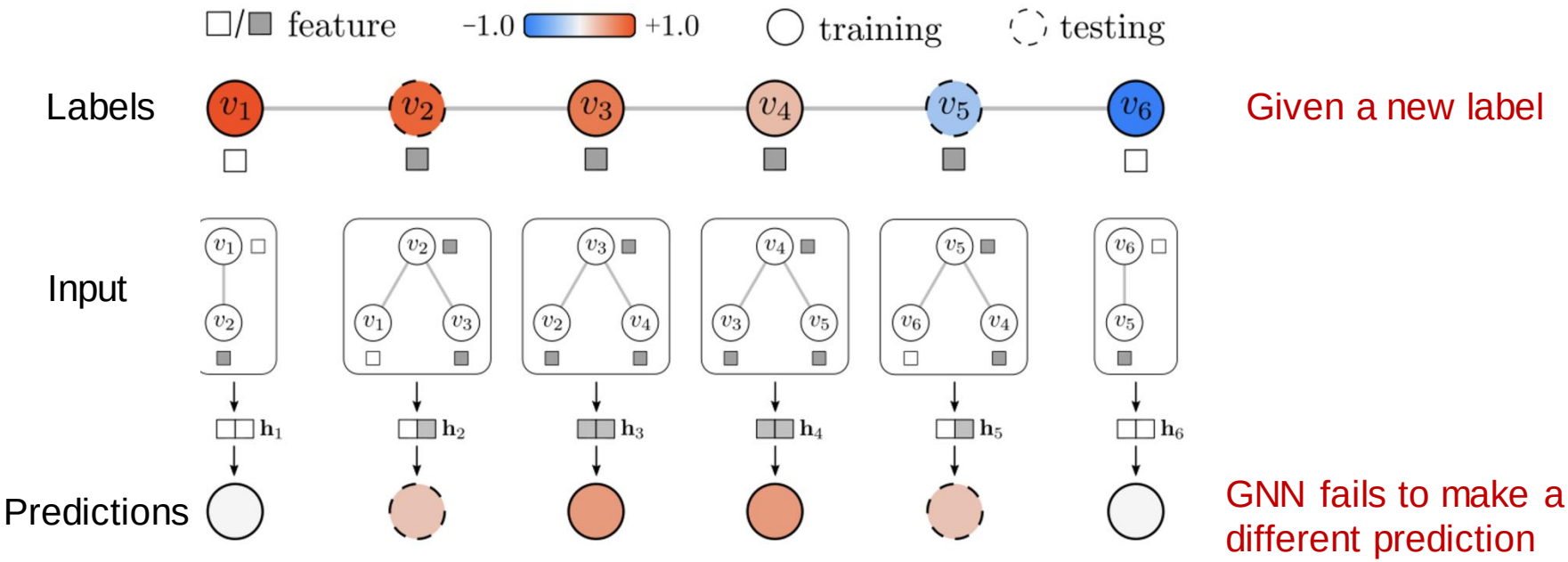
1. Form local neighborhoods.
2. Combine features to get a representation h_V at node v.
3. Predict outcome given representation (learn params with train data).

If node features are overwhelmingly predictive, making uncorrelated predictions for each node is OK.

[Adapted from "Label Propagation and Graph Neural Networks"]

GNNs make uncorrelated predictions

Uncorrelated GNN predictions can be catastrophic in simple cases **when features are only mildly predictive.**

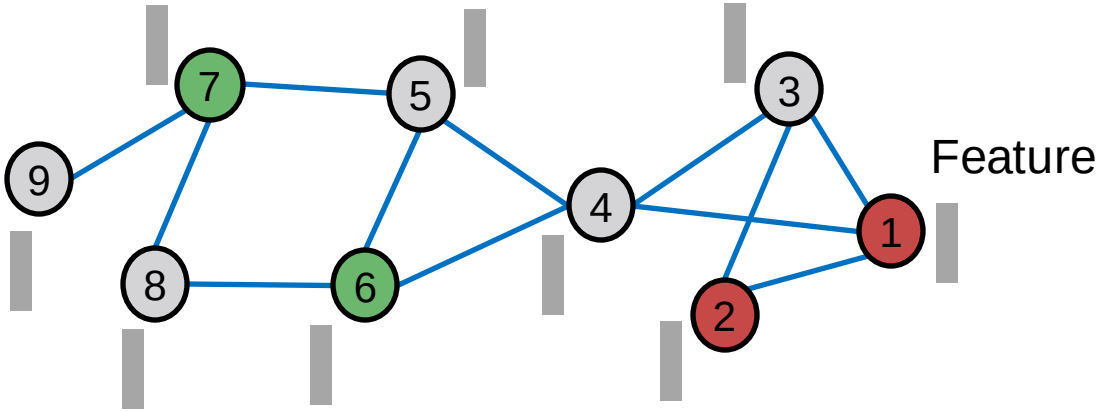


- **Big problem!** Features are no longer super predictive.
- LP (ignoring features) would work much better.

Correct & Smooth

[Huang et al., ICLR 2021]

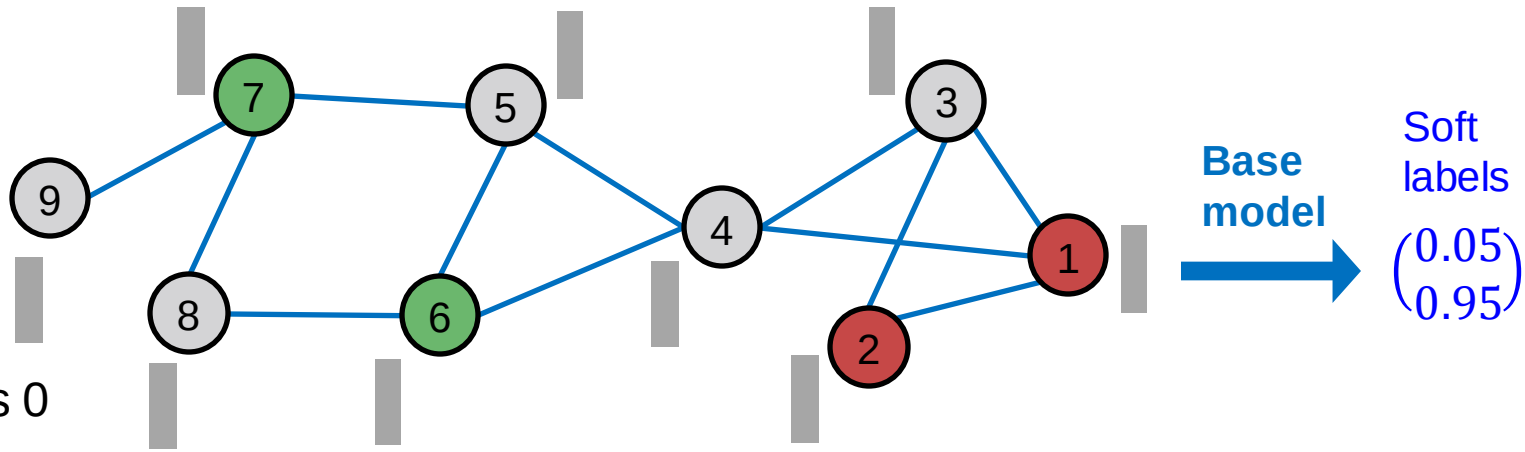
- **Setting:** A partially labeled graph and features over nodes.



- **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

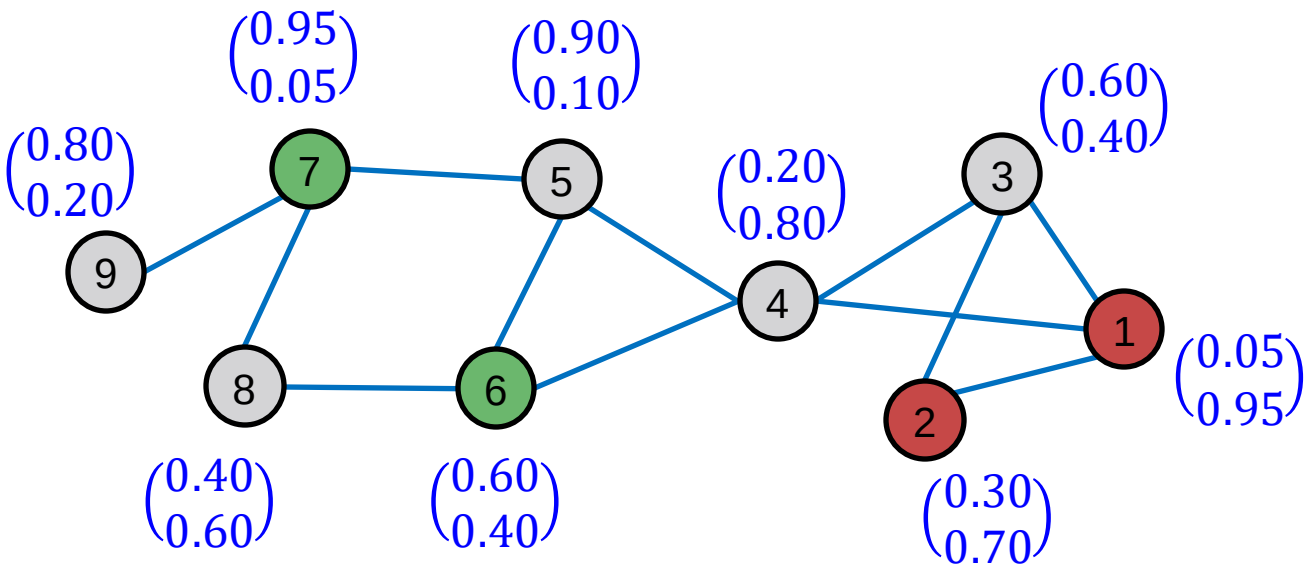
- **(1) Train a base predictor that predict soft labels (class probabilities) over all nodes.**
  - Labeled nodes are used for train/validation data.
  - Base predictor can be simple:
    - Linear model/Multi-Layer-Perceptron(MLP) over node features, or a full GNN



Green: Class 0
Red: Class 1

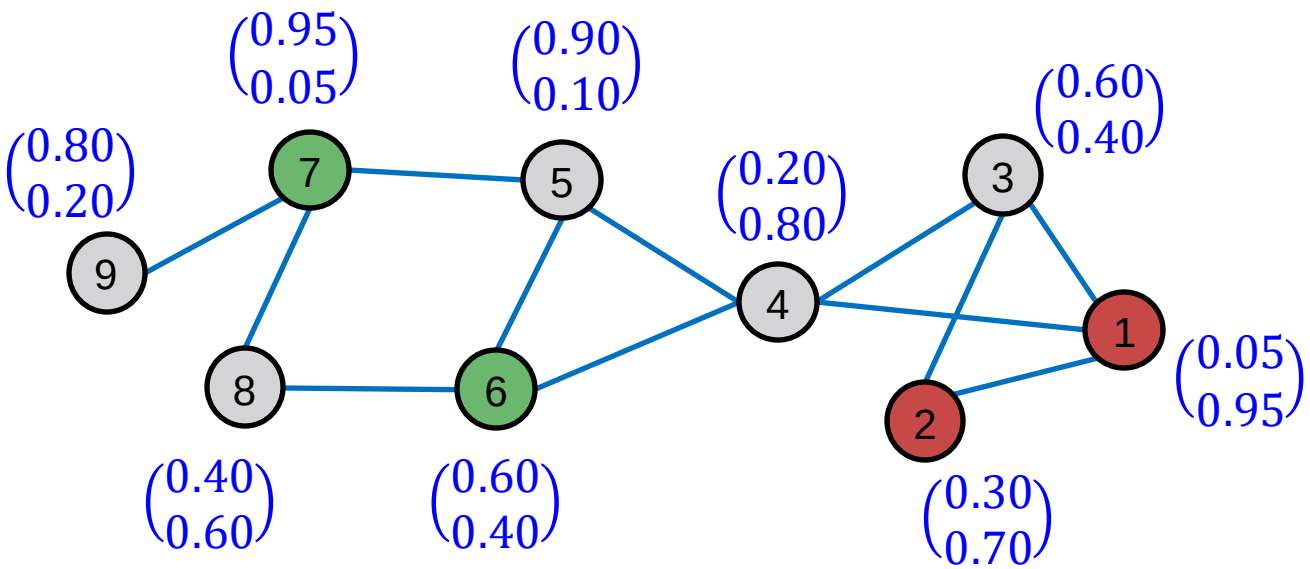
C&S: (2) Predict Over All Nodes

- **(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?**



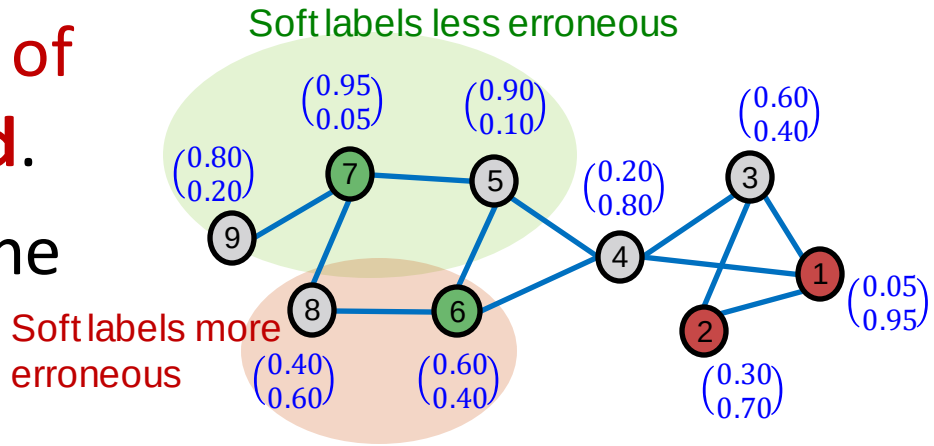
C&S: (3) Post-Process Predictions

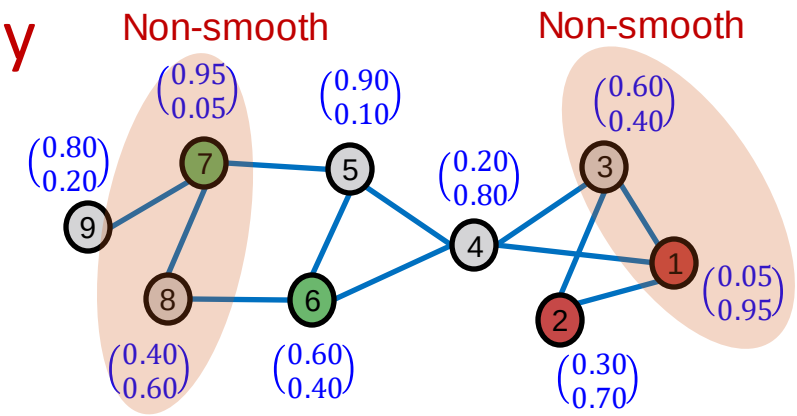
- **(3) C&S uses the 2-step procedure to post-process the soft predictions.**
  1. **Correct step**
  2. **Smooth step**



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.



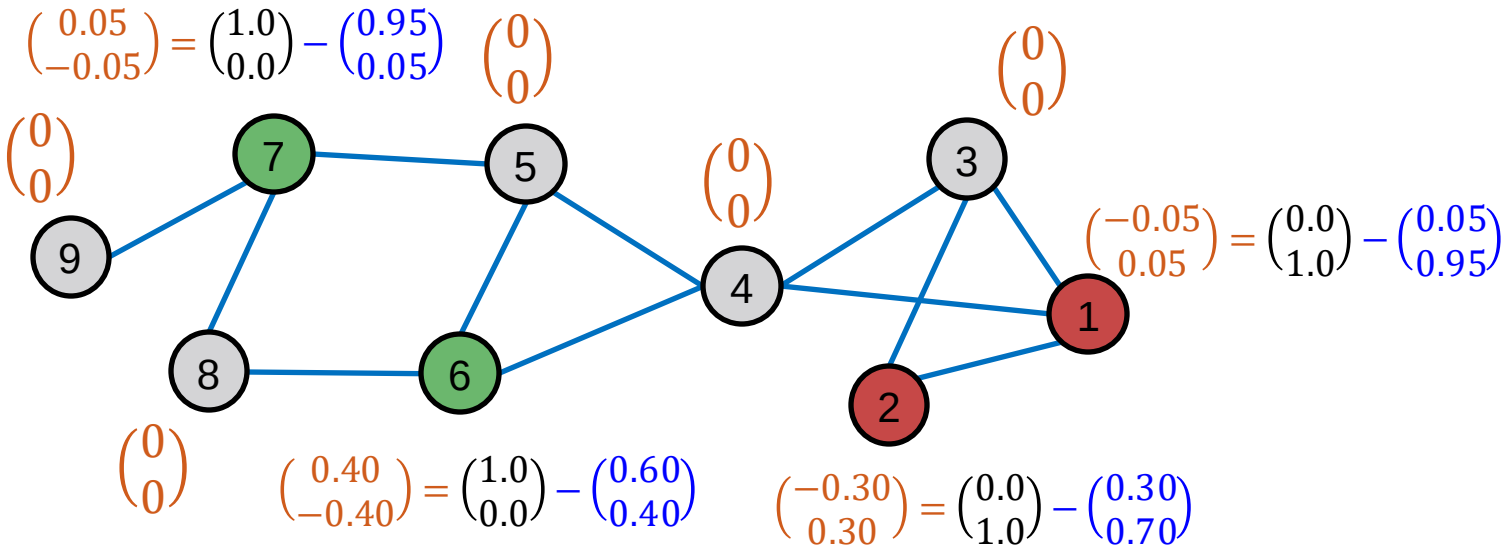


C&S Post-Processing: Correct Step

- 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.

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.



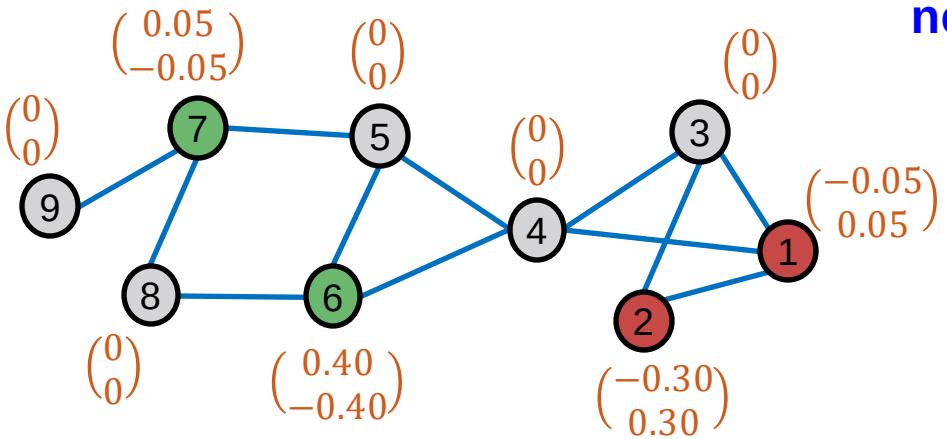
C&S Post-Processing: Correct Step (2)

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

Hyper-parameter

Diffuse training errors along the edges

Assumption: errors are similar for nearby nodes

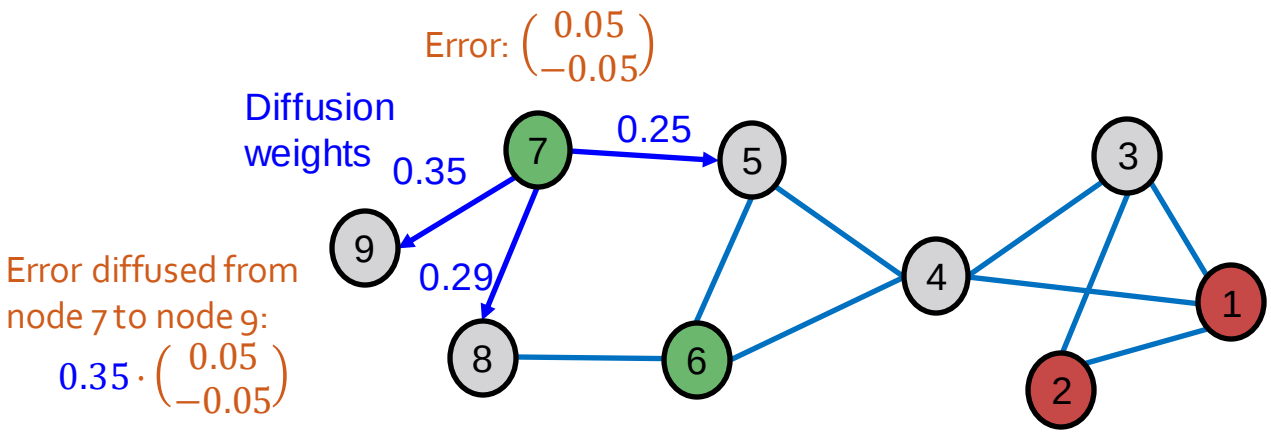


Initial training error matrix

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

Diffusion Matrix $\tilde{A}$

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

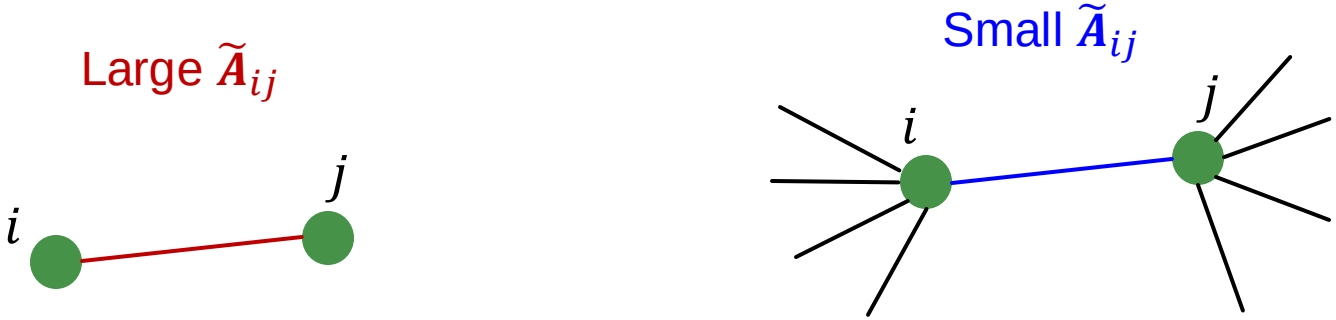


Theoretical Motivation for $\tilde{A}$

- **Normalized diffusion matrix $\tilde{A} \equiv D^{-1/2}AD^{-1/2}$**
- All the eigenvalues λ'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: $\tilde{A}D^{1/2}\mathbf{1} = D^{-1/2}AD^{-1/2}D^{1/2}\mathbf{1} = D^{-1/2}A\mathbf{1} = D^{-1/2}D\mathbf{1} = 1 \cdot D^{1/2}\mathbf{1}$.
      - $A\mathbf{1} = D\mathbf{1}$, since they both leads to node degree vector
  - The power of $\tilde{A}$ (i.e., $\tilde{A}^K$) is **well-behaved for any K**.
    - The eigenvalues of $\tilde{A}^K$ are always within [-1,1].
    - The largest eigenvalue is always 1.
    - Output of $\tilde{A}x$ (e.g., in error diffusion) is **normalized**

More Intuitions 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)

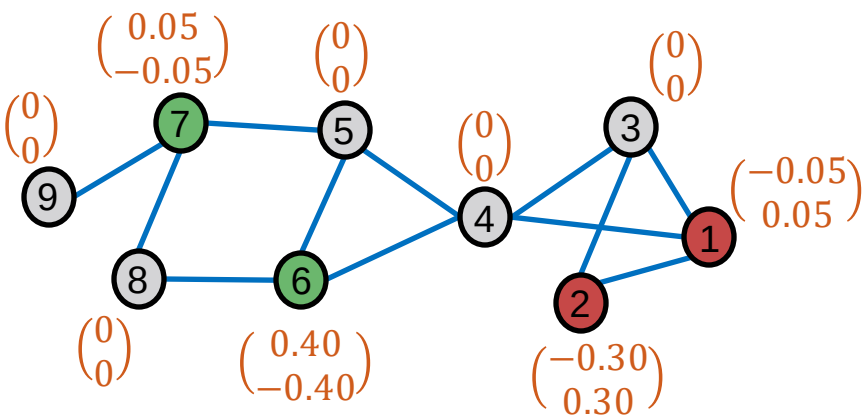
- **Diffusion of training errors:**

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

Assumption: Prediction errors are similar for nearby nodes.

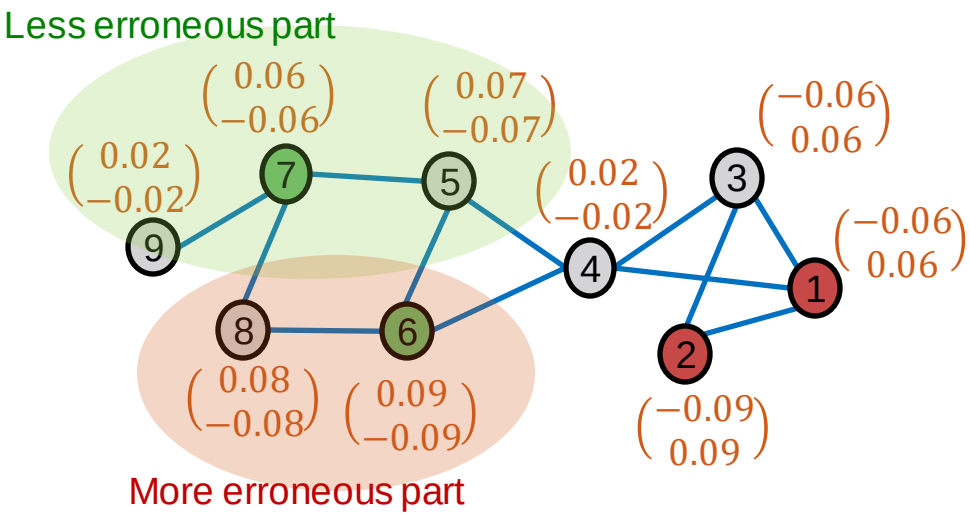
Before diffusion

$\boldsymbol{E}^{(0)}$



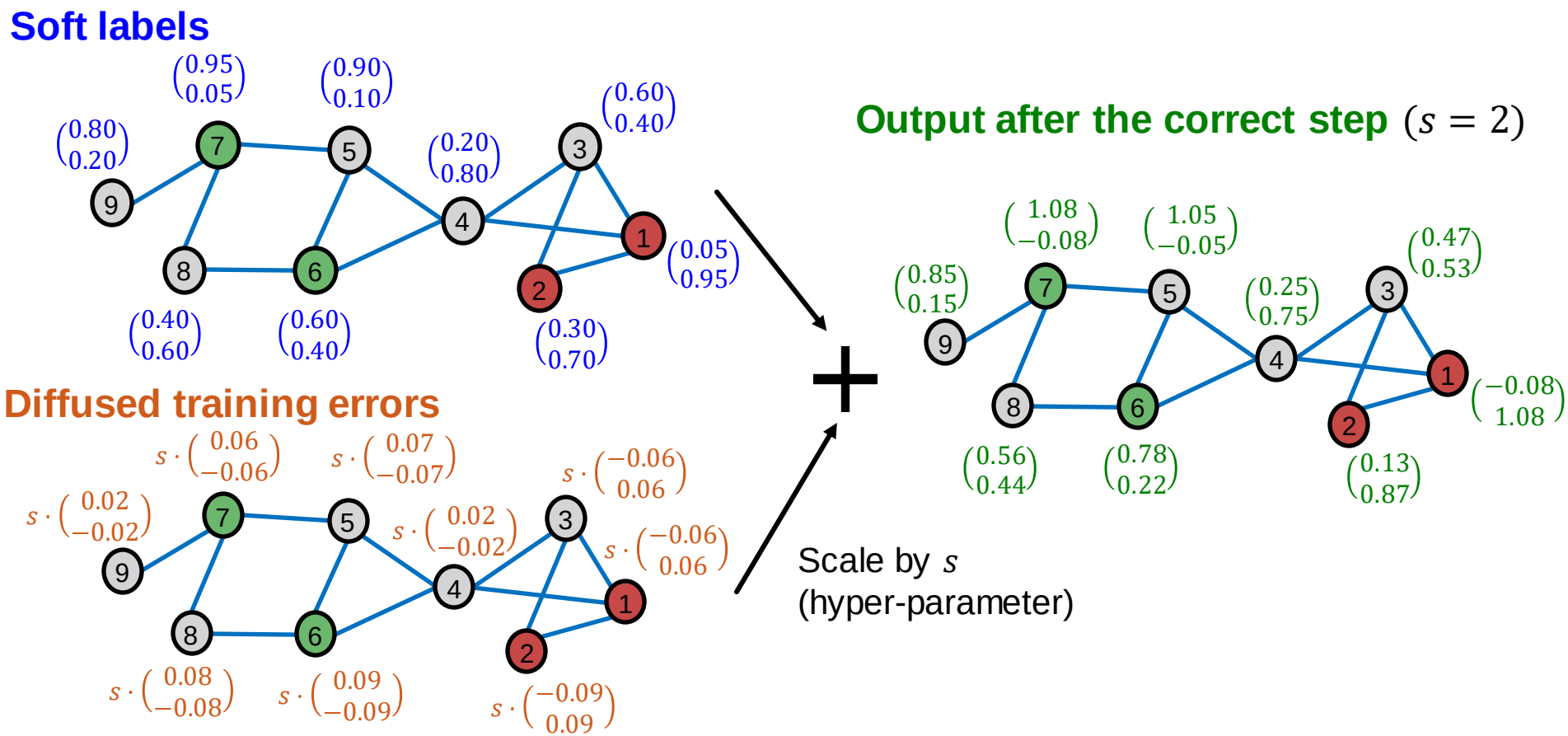
After diffusion

$\boldsymbol{E}^{(3)}, \alpha = 0.8$



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

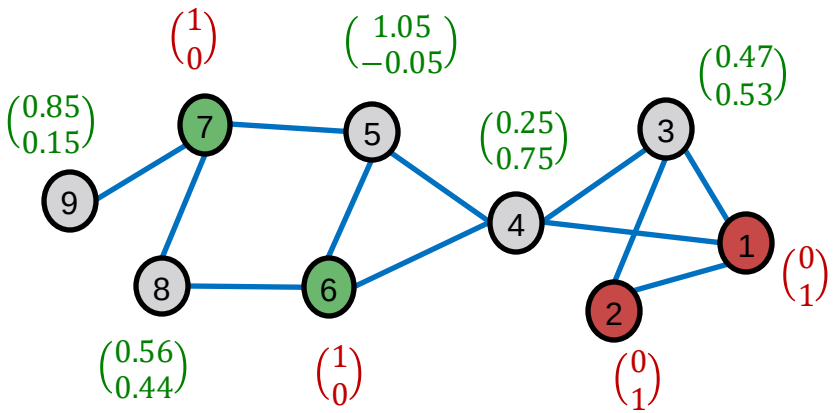
- **Add the scaled diffused training errors into the predicted soft labels**



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:

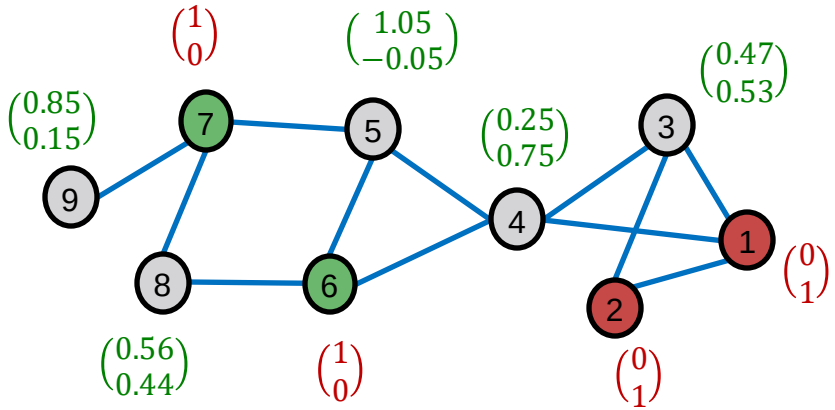


C&S Post-Processing: Smooth Step (1)

- **Smooth step:**
  - Diffuse label $\boldsymbol{Z}^{(0)}$ along the graph structure.
  - $Z^{(t+1)} \leftarrow (1 - \alpha) \cdot Z^{(t)} + \alpha \cdot \tilde{\boldsymbol{A}} Z^{(t)}$.

Hyper-parameter

Diffuse labels along the edges



Corrected label matrix

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

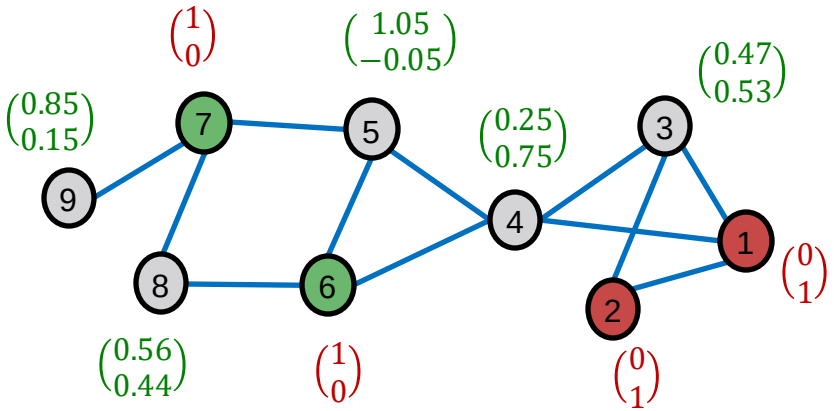
C&S Post-Processing: Correct Step (2)

- **Smooth step:**

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

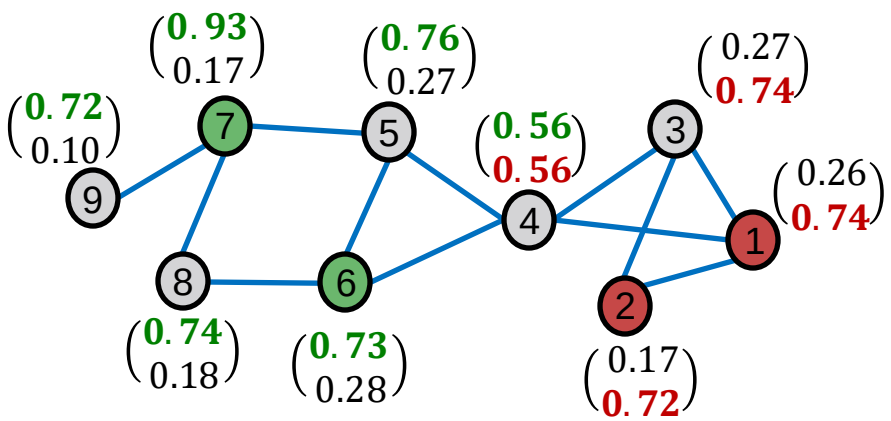
Before smoothing

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



After smoothing

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



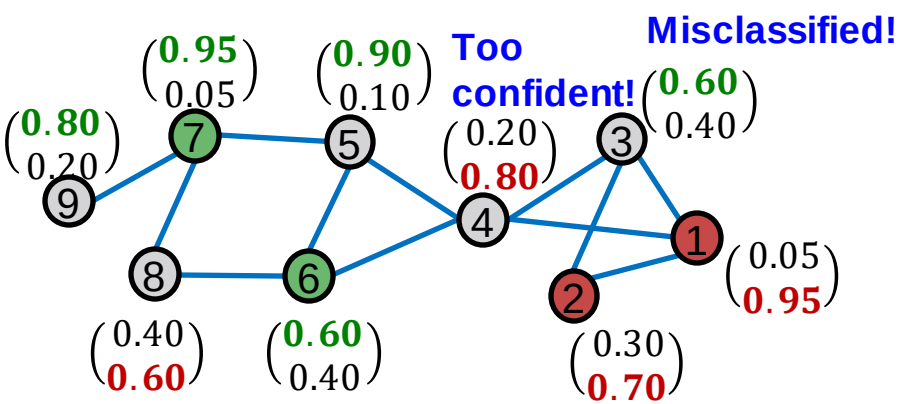
The final class prediction of C&S is the class with the maximum $\boldsymbol{Z}^{(3)}$ score.

Note: The $\boldsymbol{Z}^{(3)}$ 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.

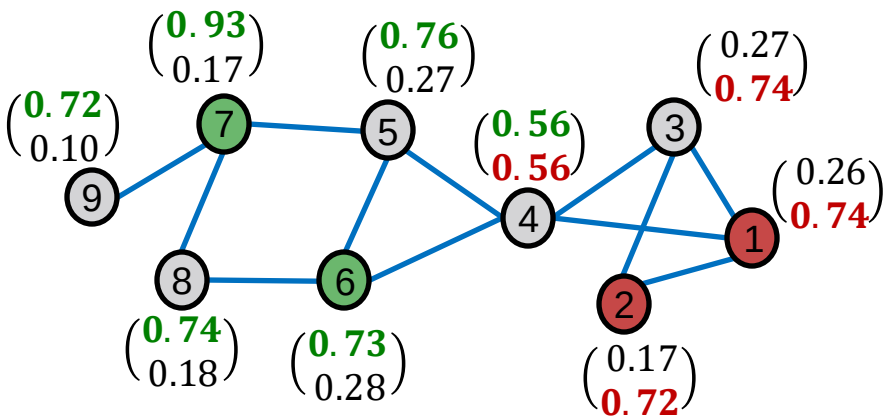
C&S: Toy Example Summary

- 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 (*e.g.,* 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
MLP + C&S	**84.18**

Correct & Smooth: Summary

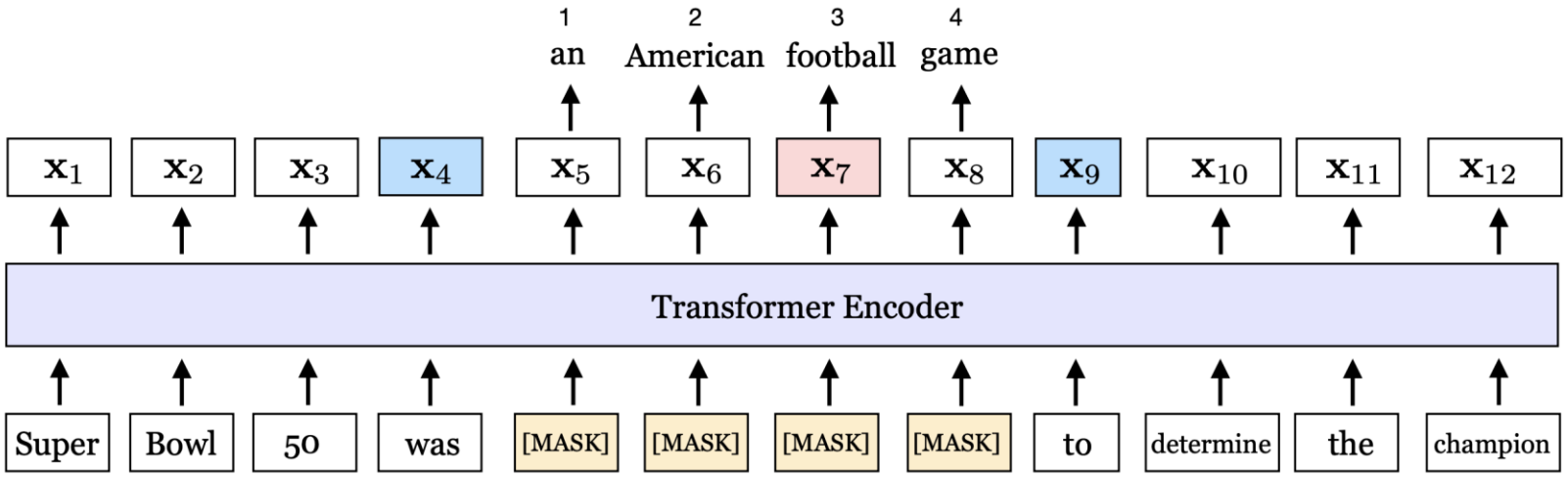
- Correct & Smooth (C&S) **uses graph structure to post-process** the soft node labels predicted by any base model.
- **Correction step**: Diffuse and correct for the training errors of the base predictor.
- **Smooth step**: Smoothen the prediction of the base predictor (a variant of **label propagation**).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

Stanford CS224W: Masked Label Prediction

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

Masked Label Prediction

- An alternative approach to **explicitly include node label information** (works with GNN).
- Inspired from BERT objective in NLP.
  - Pretraining strategy: **masked word prediction**



Masked Label Prediction

[Shi et al., IJCAI 2021]

- **Idea: Treat labels as additional features**
  - Concatenate the **node label matrix** Y with the **node feature matrix** X
- **ML setting**: Use **partially observed labels** $\hat{Y}$ to predict the **remaining unobserved labels**
  - **Training:** First corrupt $\hat{Y}$ into $\tilde{Y}$ by randomly masking a portion of node labels to zeros, then use $[X, \tilde{Y}]$ to predict the masked node labels.
  - **Inference:** Employ all $\hat{Y}$ to predict the remaining unlabeled nodes (in the validation/test set).
  - **Similar to link prediction!** Also a self-supervised task

Summary of the Lecture

- We discussed 3 ideas that **explicitly use labels** when making predictions on graphs
  - **Label propagation**
    - Directly propagate known labels to all the nodes
  - **Correct & Smooth**
    - First define a base predictor, then correct and smooth the predictions with label propagation
  - **Masked label prediction**
    - Construct a self-supervised ML task, let graph ML model to propagate label information

Summary of ML with Graphs

- We discussed 3 frameworks to approach **machine learning tasks on graphs**
- **Node embeddings**
  - Embed nodes into Euclidean space, and use distance metric in embedding space to approximate node similarity
- **Graph Neural Networks**
  - Iterative neighborhood aggregation
- **Label Propagation**
  - Inductive bias: homophily
  - Explicitly incorporate label information when making predictions