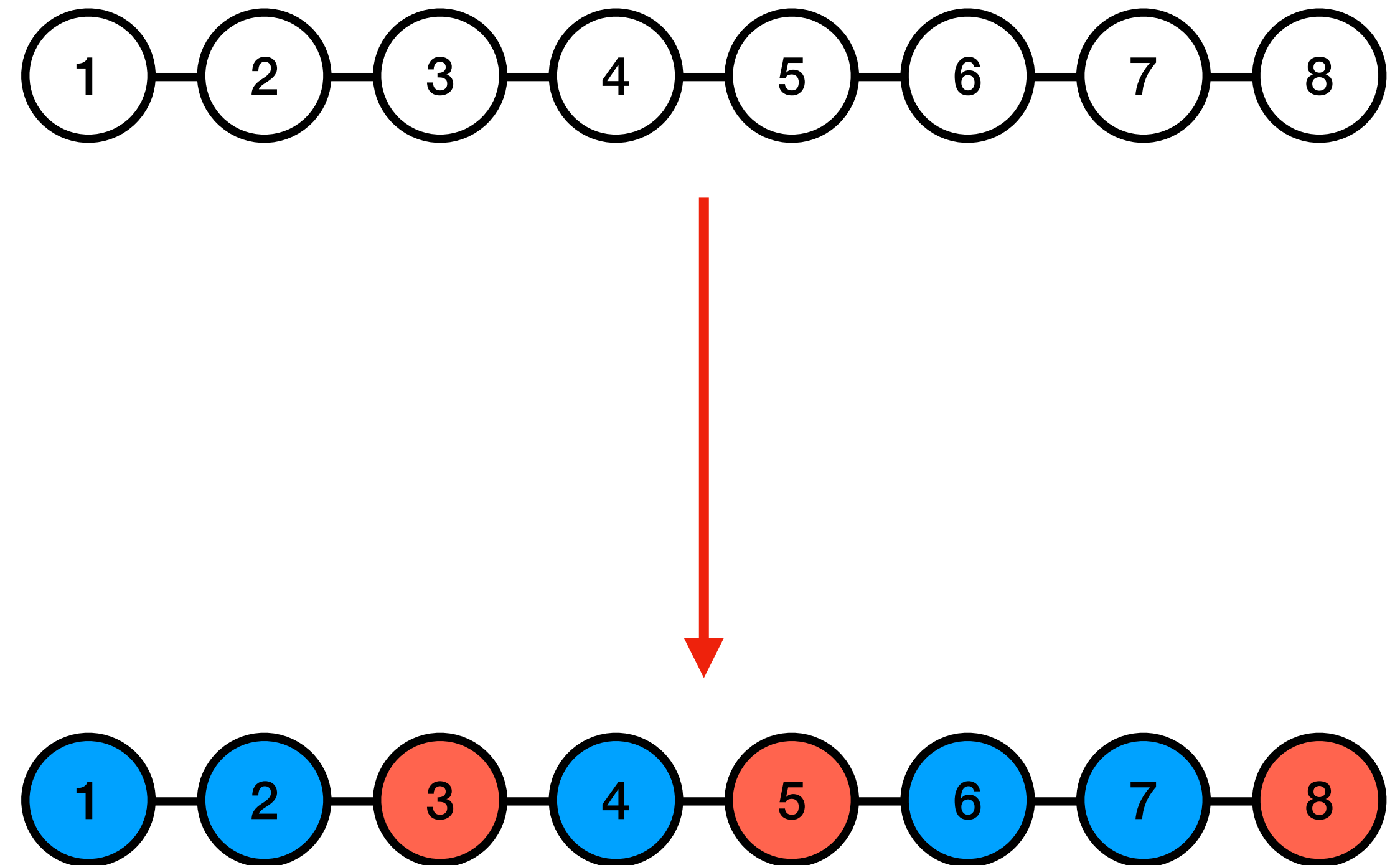


# **GALAXY: Graph-based Active Learning at the Extreme**

*Jifan Zhang, Julian Katz-Samuels, Robert Nowak*  
University of Wisconsin, Madison

# Graph-based Active Learning

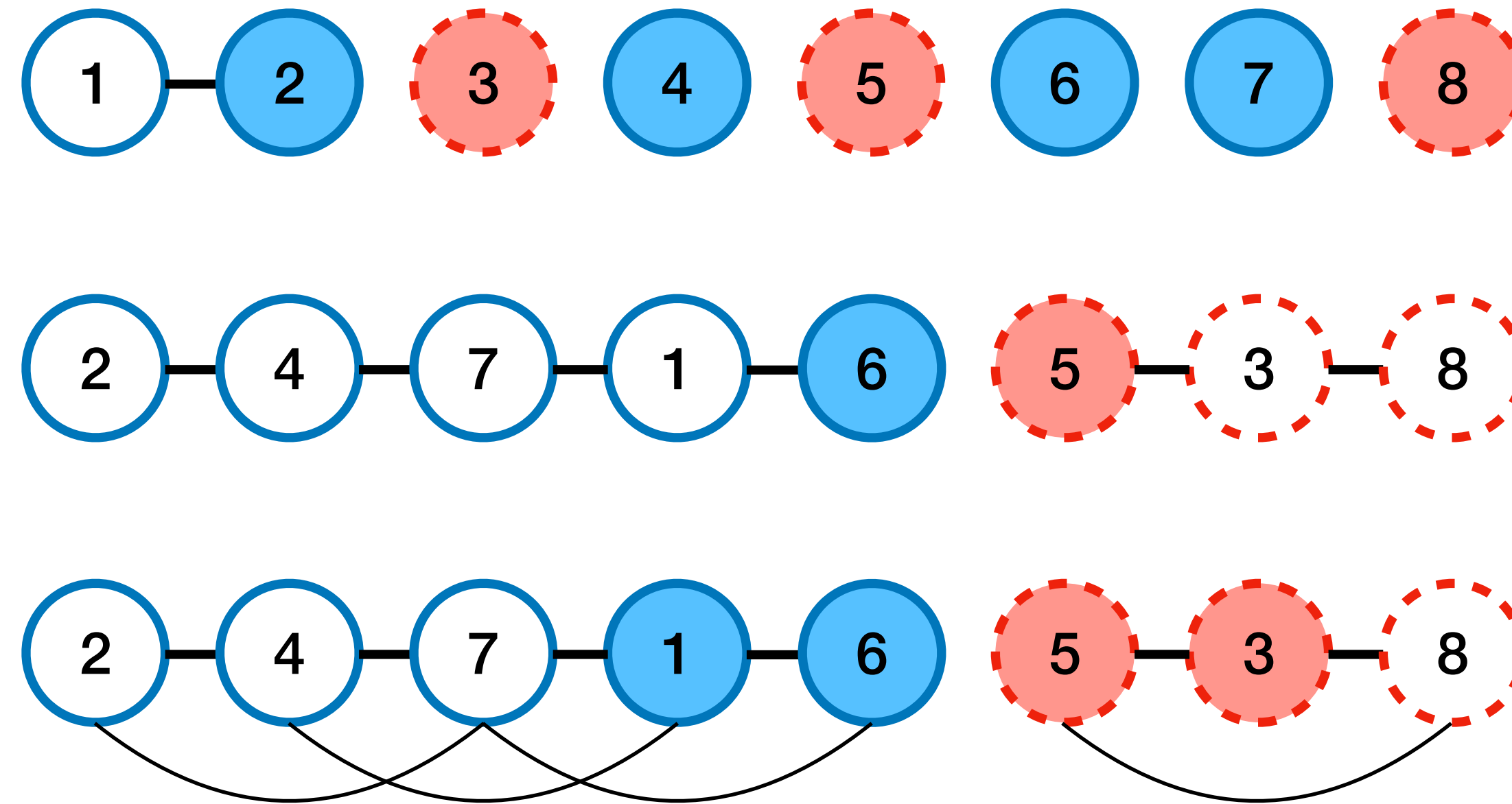
- Given a pool of unlabeled examples  $X$ , annotation cost is expensive
- Each example  $x_i$  is a node in graph  $G = (X, E)$
- Each example has its corresponding label  $f^*(x_i)$
- **Objective: annotate as few examples as possible for a classifier to reach 100% accuracy.**



# Insight from $\mathcal{S}^2$

[Dasarathy, Nowak & Zhu, ICML 2015]

- Not all graphs are equally difficult (sample complexity) to learn.



**Can we simultaneously learn  
good classifiers and better graphs?**

# Leveraging a Deep Neural Network

## Construct\_Graph

Input: Pool  $X$ , number of classes  $K$ , neural network

$$f_{\theta} : \mathcal{X} \rightarrow \Delta^{(K-1)}$$

Initialize: Confidence for each  $i \in [N]$ :

$$q_i \leftarrow \max_{k \in [K]} [f_{\theta}(x_i)]_k$$

For  $k = 1, \dots, K$ :

Sort examples by margin scores

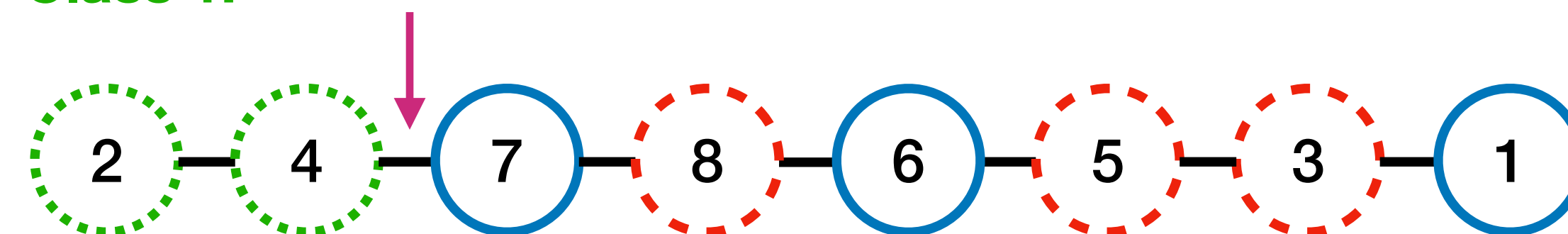
$$\delta_i^{(k)} \leftarrow [f_{\theta}(x_i)]_k - q_i \text{ and break tie by } q_i$$

Construct linear edge set  $E^{(k)}$  connecting the sorted examples

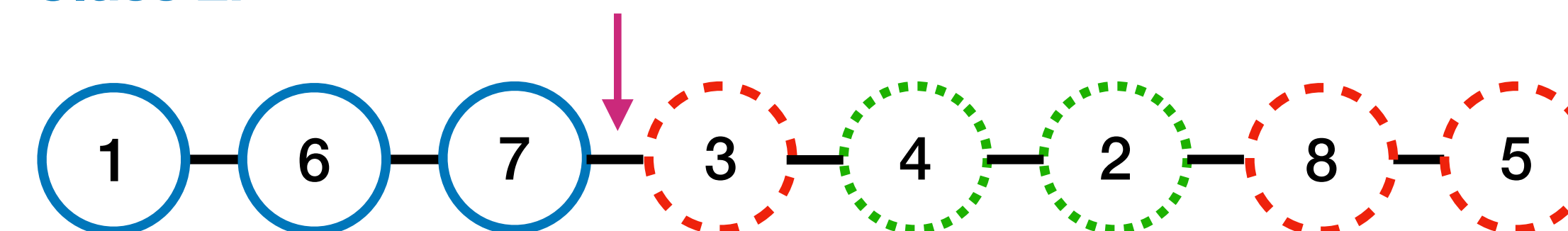
Return: Graphs  $\{G^{(k)} = (X, E^{(k)})\}_{k=1}^K$

When  $f_{\theta}$  is a perfect classifier

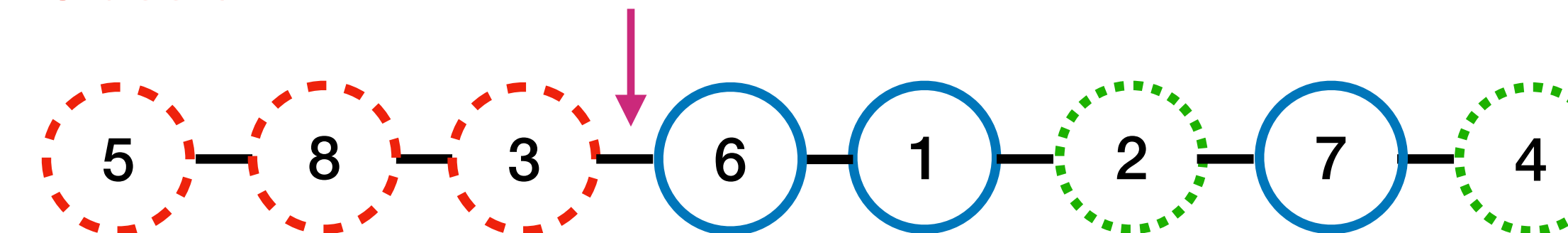
Class 1:



Class 2:



Class 3:



Low margin score

High margin score



# Leveraging a Deep Neural Network

## Construct\_Graph

Input: Pool  $X$ , number of classes  $K$ , neural network

$$f_{\theta} : \mathcal{X} \rightarrow \Delta^{(K-1)}$$

Initialize: Confidence for each  $i \in [N]$ :

$$q_i \leftarrow \max_{k \in [K]} [f_{\theta}(x_i)]_k$$

For  $k = 1, \dots, K$ :

Sort examples by margin scores

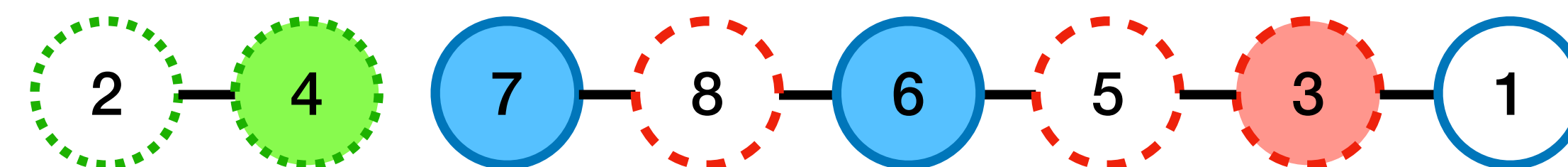
$$\delta_i^{(k)} \leftarrow [f_{\theta}(x_i)]_k - q_i \text{ and break tie by } q_i$$

Construct linear edge set  $E^{(k)}$  connecting the sorted examples

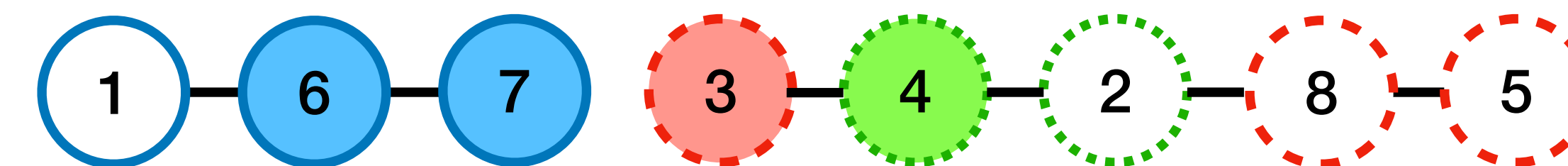
Return: Graphs  $\{G^{(k)} = (X, E^{(k)})\}_{k=1}^K$

Idea: Bisect to find one-vs-all cuts

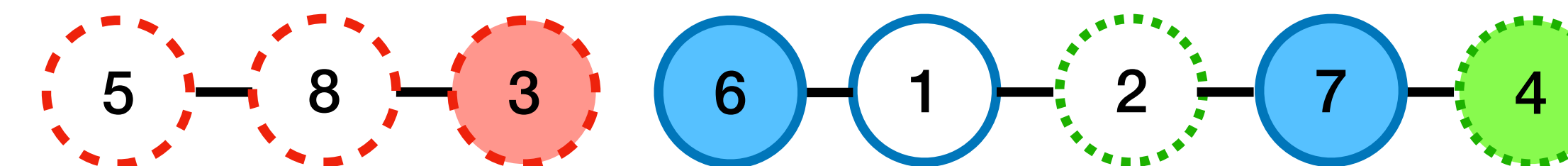
Class 1:



Class 2:



Class 3:



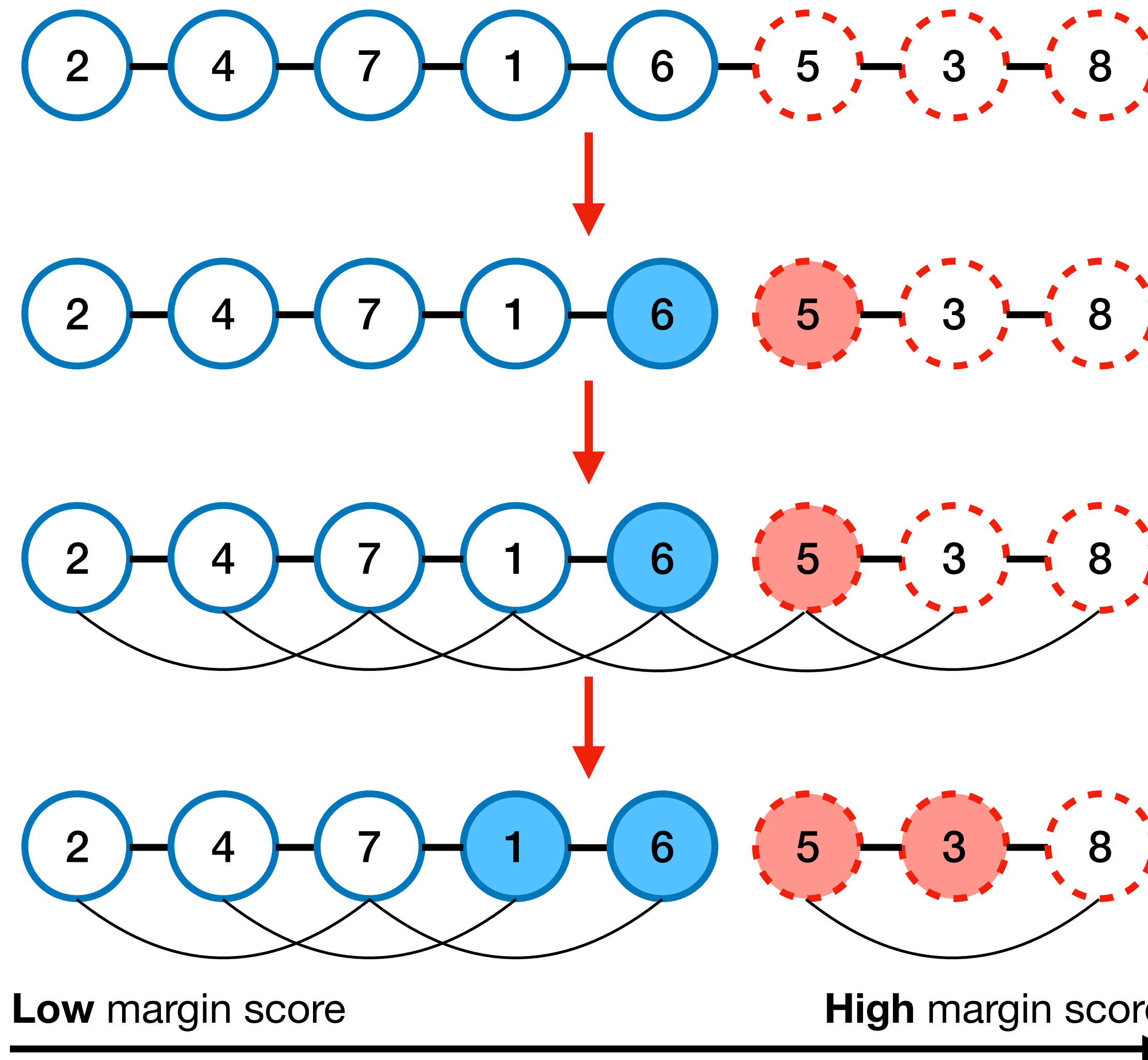
Low margin score

High margin score



# GALAXY in Separable Case

= Bisection + Querying Around Uncertainty Boundary



# Extreme Class Imbalance

- Define number of examples in each class:  $N_k = |\{x \in X | f^\star(x) = k\}|$
- Extreme class imbalance

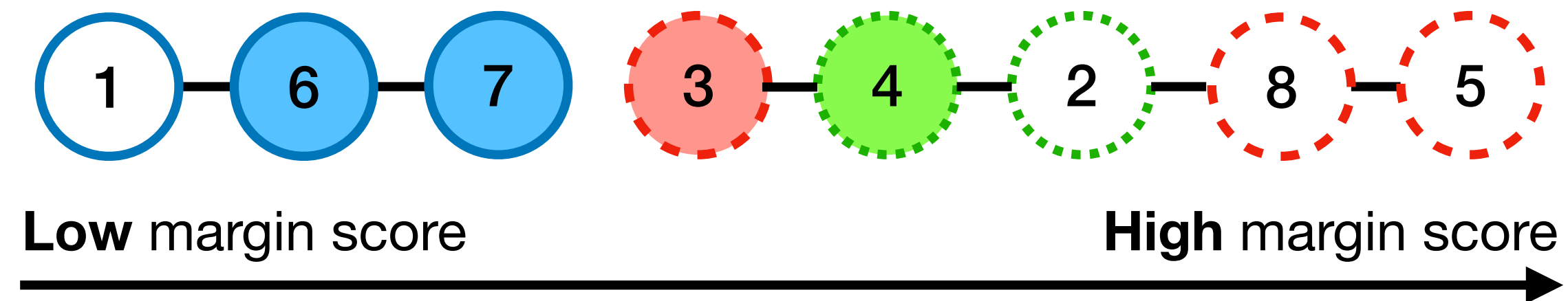
$$\frac{N_k}{N_K} \leq \epsilon, k = 1, \dots, K - 1$$

I.e., one class has significantly more examples than any other class.

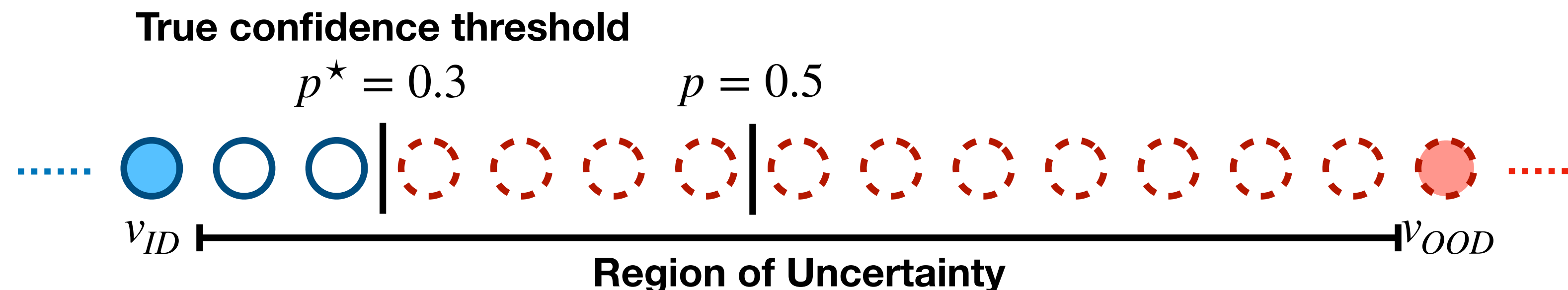


# Key Ingredients

- Annotate Uncertain Examples



- [Theorem] Annotate Class-diverse (class-balanced) Examples: lower bound on the balancedness of collected examples



- [Theorem] Uncertainty sampling in certain cases could collect **zero** minority labels on expectation.

# Experiments: Extremely Unbalanced Datasets

- We modify CIFAR-10, CIFAR-100 and SVHN datasets.
  - If  $K$  classes in total, then class  $1, \dots, K - 1$  are the original classes while class  $K$  includes the rest of the original dataset.
  - For example, for CIFAR-100 with 3 classes, we have classes 1 vs 2 vs 3~100.

# Experiments: Extremely Unbalanced Datasets

NAME	# CLASSES	$N_K$	$\sum_{k=1}^{K-1} N_k$	$\epsilon$
CIFAR-10	2	45000	5000	.1111
CIFAR-10	3	40000	10000	.1250
CIFAR-100	2	49500	500	.0101
CIFAR-100	3	49000	1000	.0102
CIFAR-100	10	40500	9500	.0123
SVHN	2	68309	4948	.0724
SVHN	3	54448	18809	.2546
PATHMNIST	2	80595	9401	.1166

*Table 1.* Dataset details for each extremely unbalanced scenario.  $N_K$  denotes the number of images in the out-of-distribution class while  $\sum_{k=1}^{K-1} N_k$  is the total number of images in all in-distribution classes.  $\epsilon$  is the class imbalance factor defined in Section 3.

# Baselines

## Uncertainty-based

### Algorithms

Confidence Sampling [Settles, 2009]

Cluster Margin [Citovsky et al., NeurIPS 2021]

Badge [Ash et al., ICLR 2020]

BAIT [Ash et al., NeurIPS 2021]

## Class-diverse Algorithms

Most Likely Positive [Jiang et al., NeurIPS 2018; Warmuth et al., NIPS 2001; 2003]

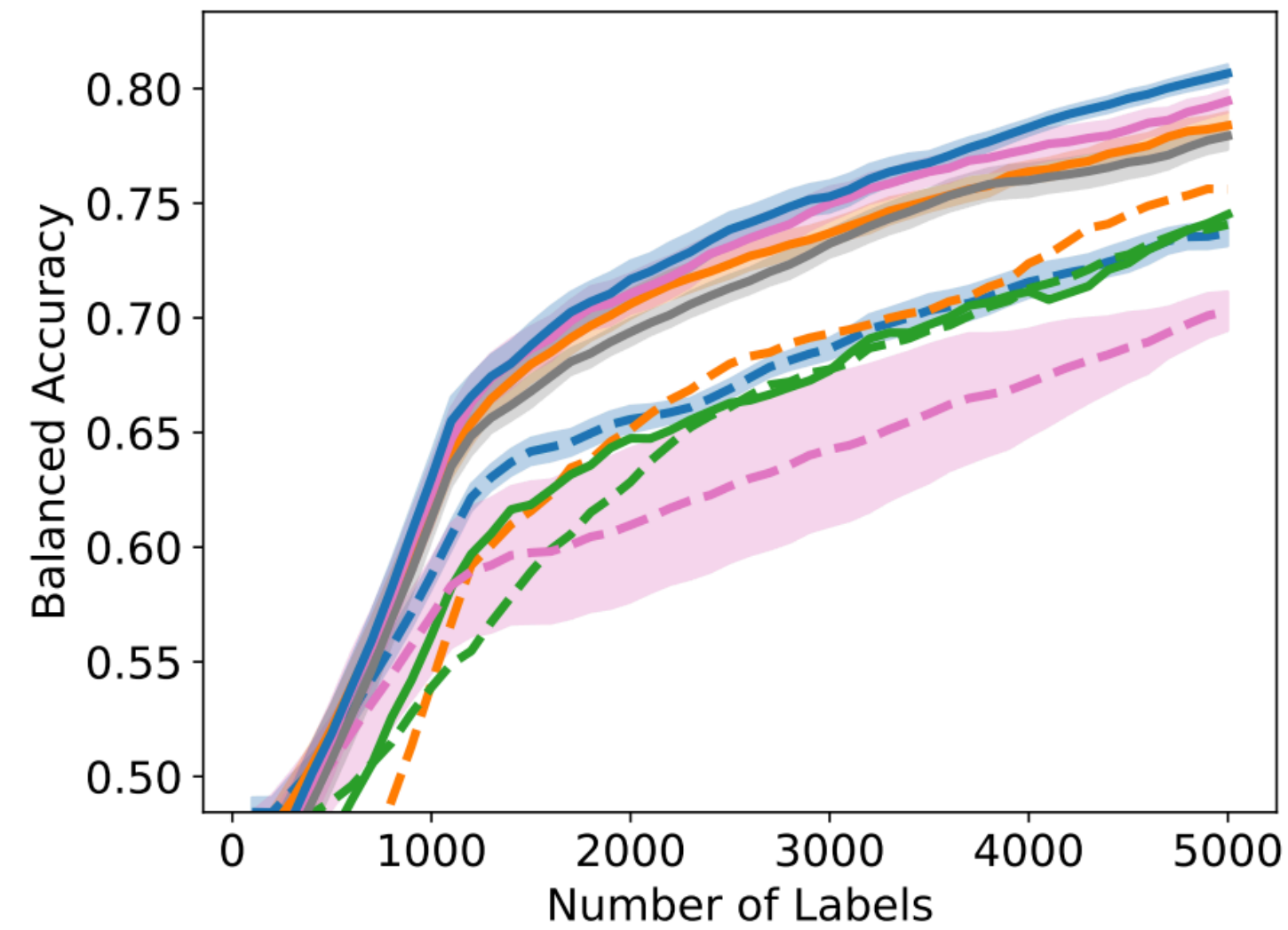
SIMILAR [Kothawade et al., NeurIPS 2021]

## Uncertainty & Class-diverse Algorithms

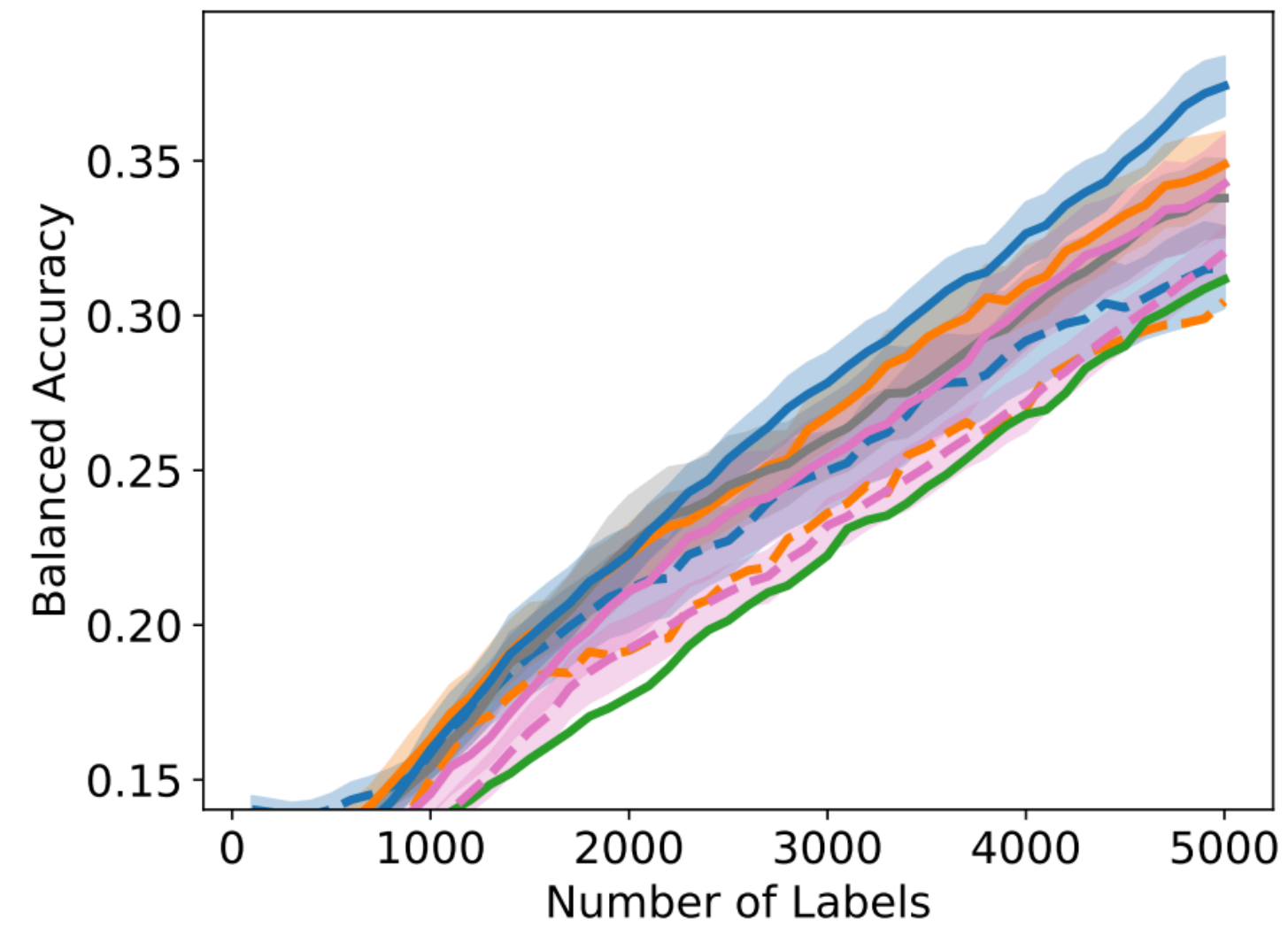
BASE [Emam, 2021]

GALAXY

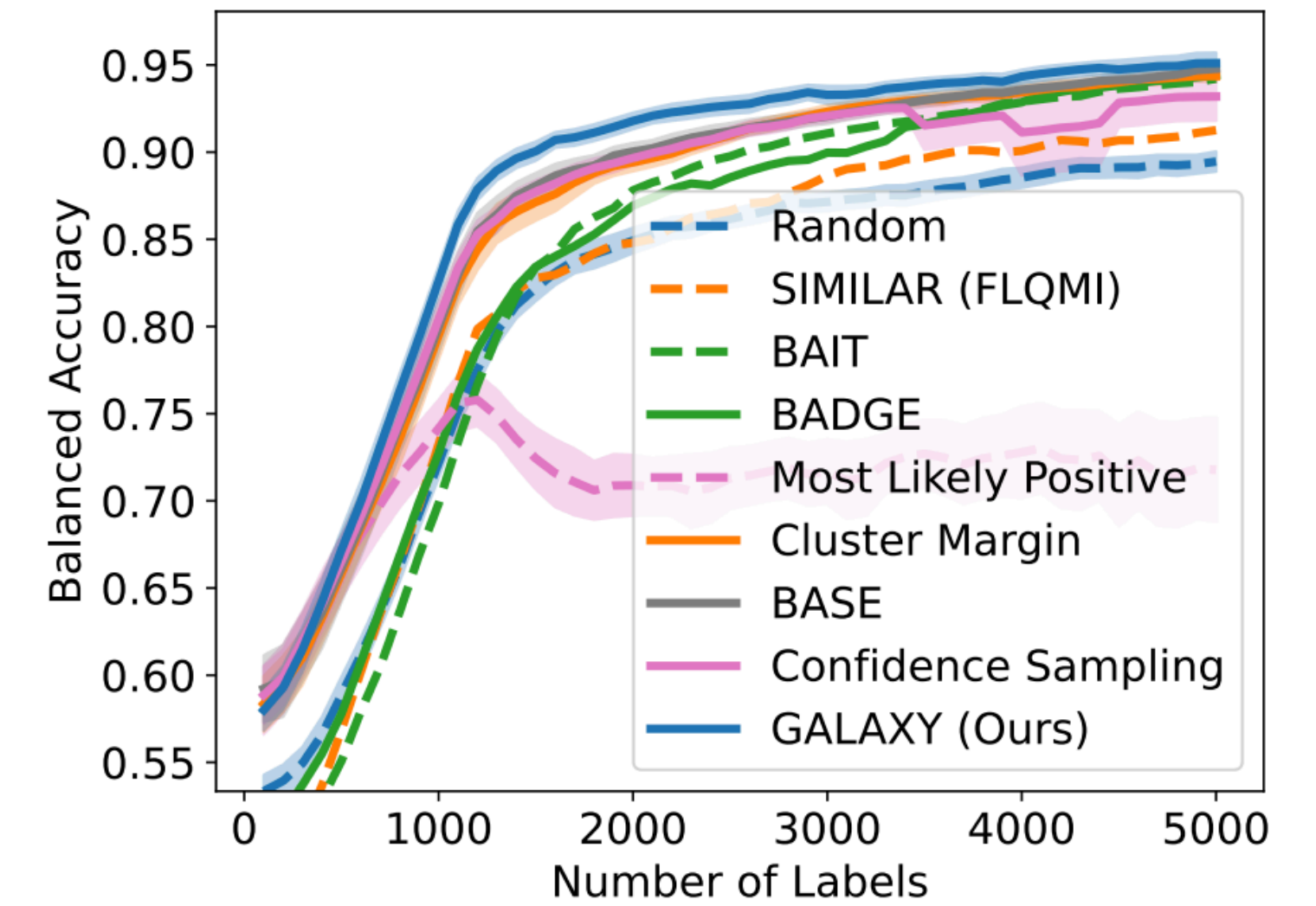
# Results: our algorithm outperforms in all settings.



(a)  $ACC_{bal}$ , CIFAR-10, 3 classes



(b)  $ACC_{bal}$ , CIFAR-100, 10 classes



(c)  $ACC_{bal}$ , SVHN, 2 classes

Figure 4. Performance of GALAXY against baselines on selected settings. Legend shown in (c) is shared across all three plots.

# Conclusion

- GALAXY vs  $S^2$ : Utilize deep neural network training to actively improve graphs.
- GALAXY vs other deep active learning
  - Finds the right uncertainty threshold and queries *uncertain* examples
  - Collects more *balanced* (class-diverse) labelled set
- Future work: Currently a batch is sequentially labelled. Can we parallelize the process to allow multiple simultaneous annotators?