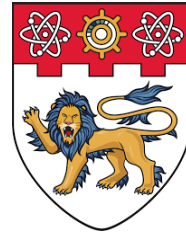


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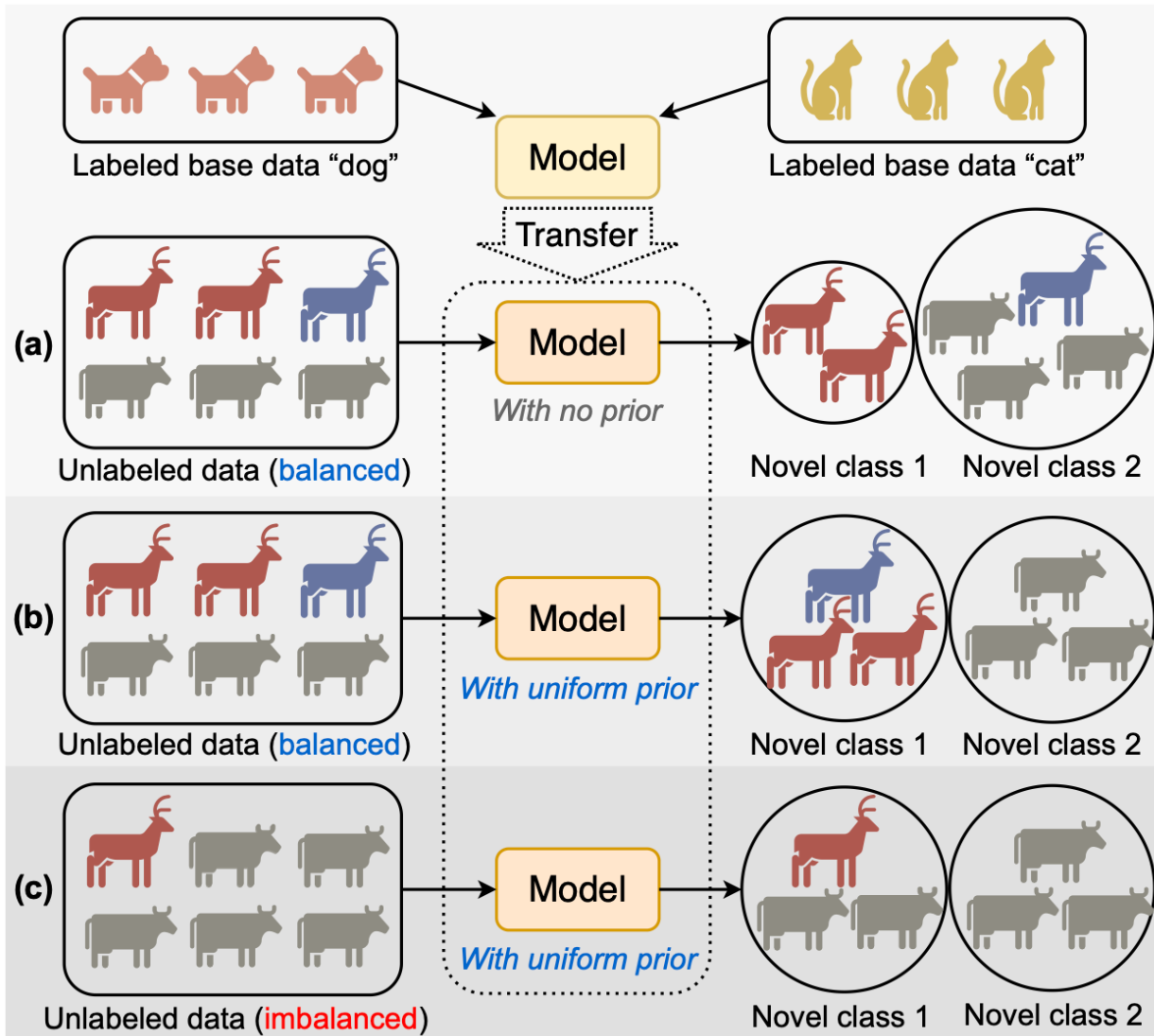
Bootstrap Your Own Prior: Towards Distribution-Agnostic Novel Class Discovery

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Introduction



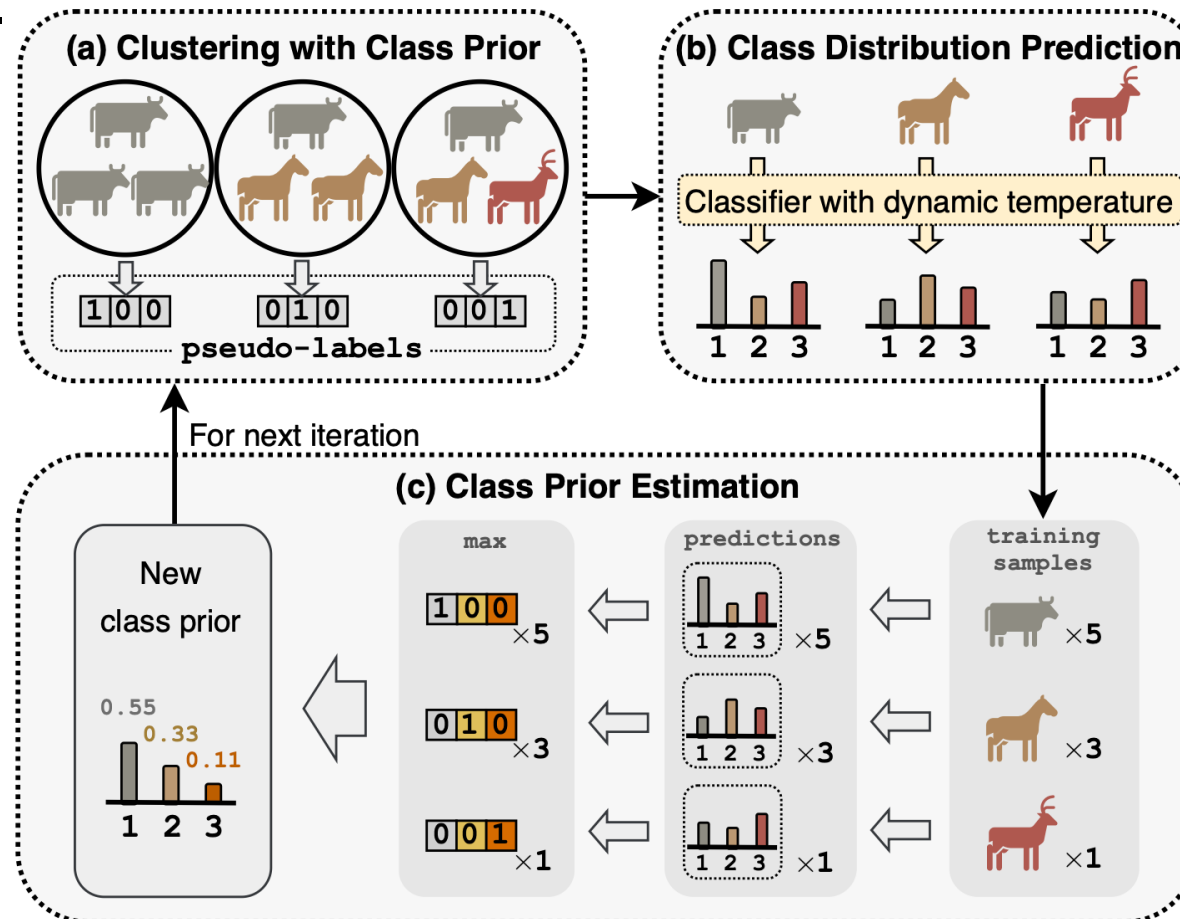
❑ An impractical assumption in existing works:
novel data is class-balanced.

We propose **Distribution-agnostic NCD**, allowing novel data drawn from arbitrary unknown class distributions

❑ The **dilemma**: class distribution prior is necessary for accurate pseudo-label generation yet is unknown in our setting.

Approach: overview

- We propose *Bootstrap Your Own Prior (BYOP)* for distribution-agnostic NCD, *i.e.*, to iteratively estimate the class distribution prior using the model prediction itself.

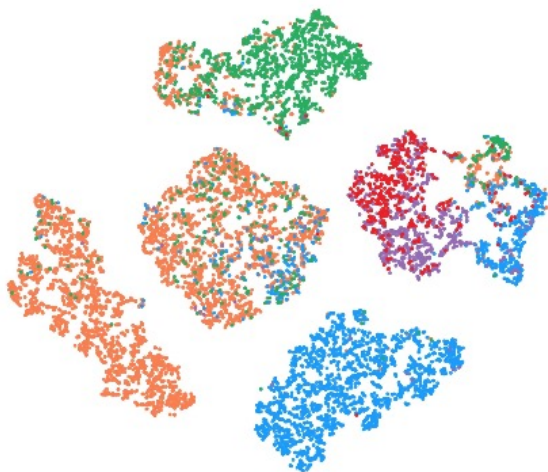


Experiments: visualizations

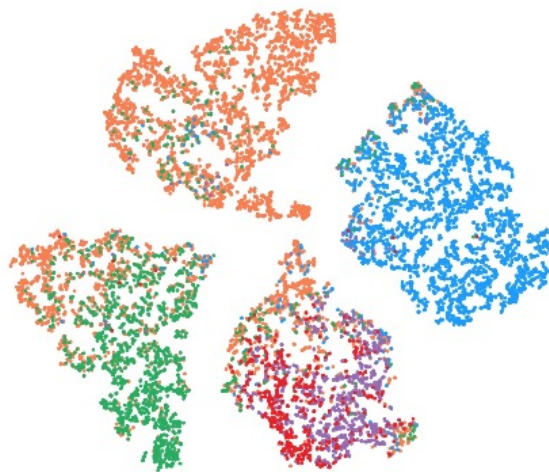
□ **Left:** t-SNE visualizations; **right:** estimated prior vs. true prior

CIFAR10 w/ imbalance ratio 10

● *dog* ● *frog* ● *horse* ● *ship* ● *truck*

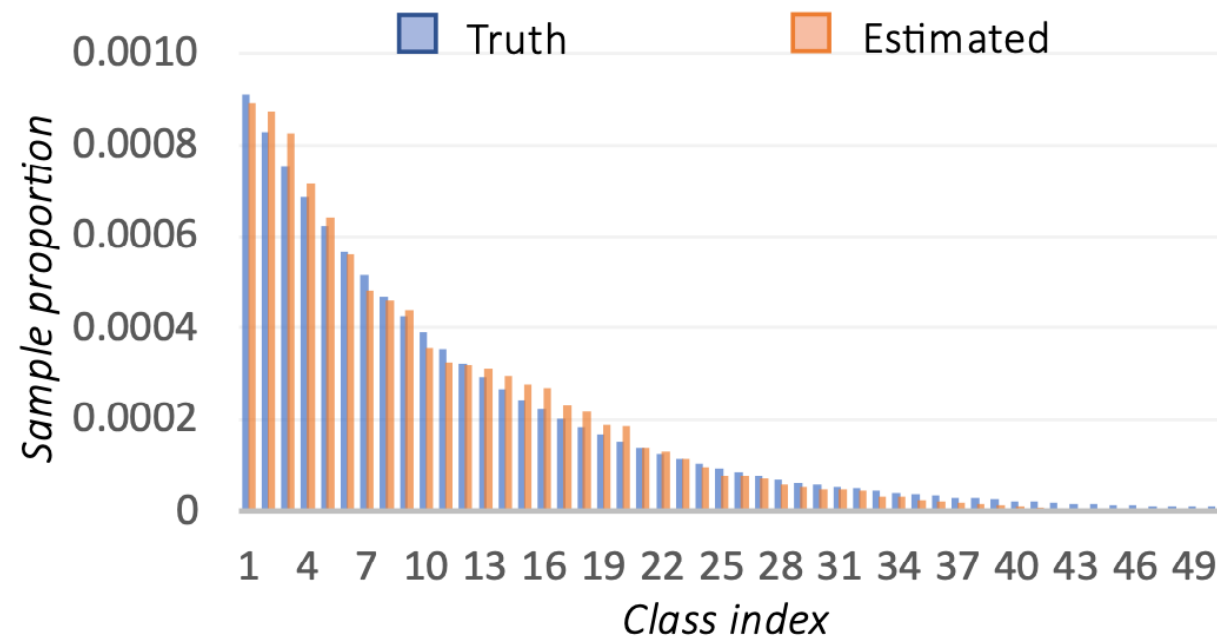


(a) UNO



(b) UNO + BYOP

CIFAR100-50 w/ imbalance ratio 100



Novel Class Discovery (NCD)

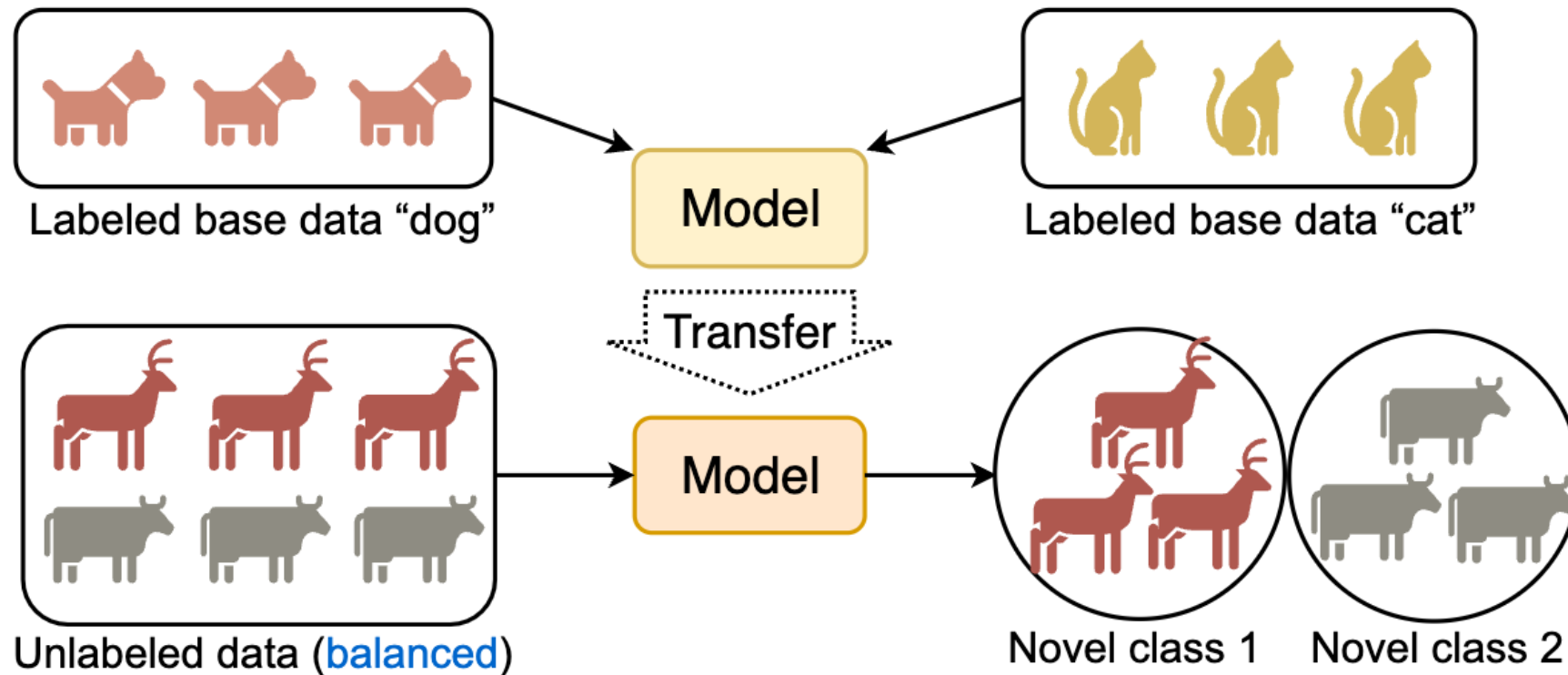
- NCD: Clustering unlabeled data according to **semantic classes** using the knowledge learned from labeled data



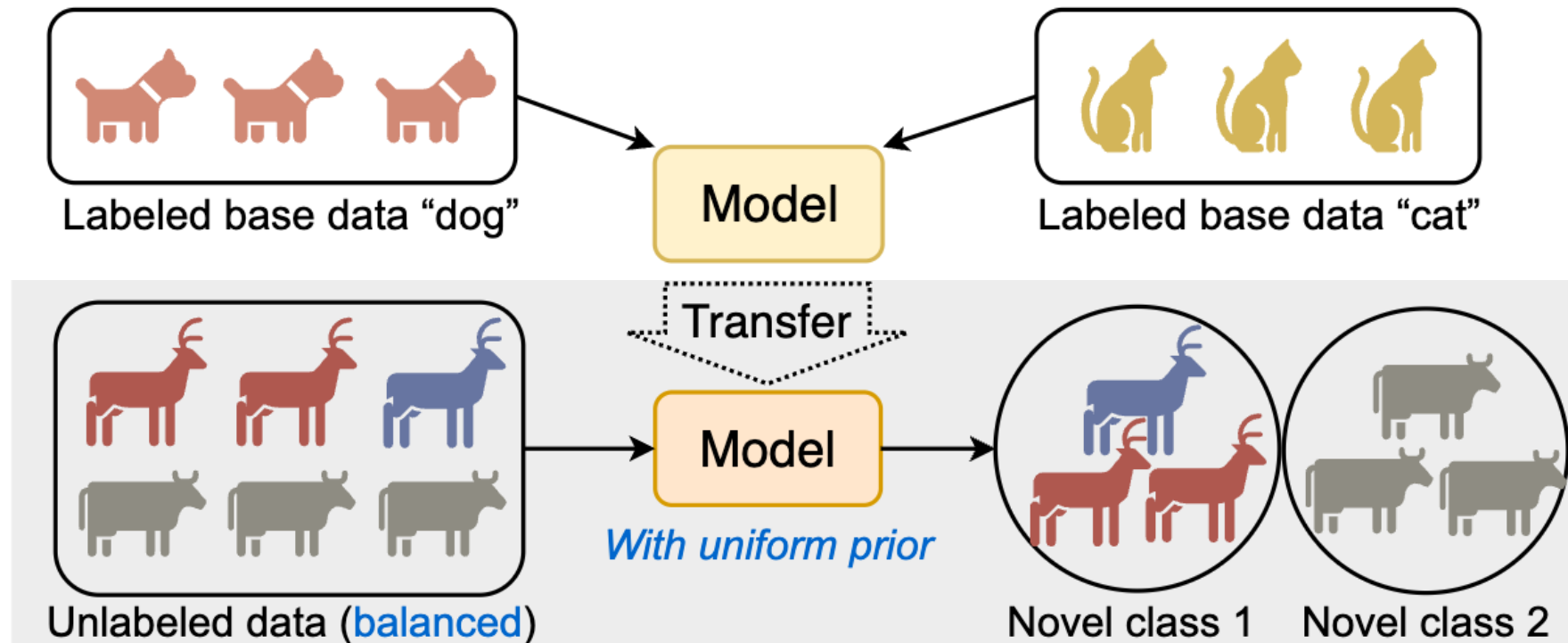
A naive solution that could be found with unsupervised clustering [1]

Introduction

- Existing works often hold a common assumption: unlabeled data has a **uniform class distribution**.

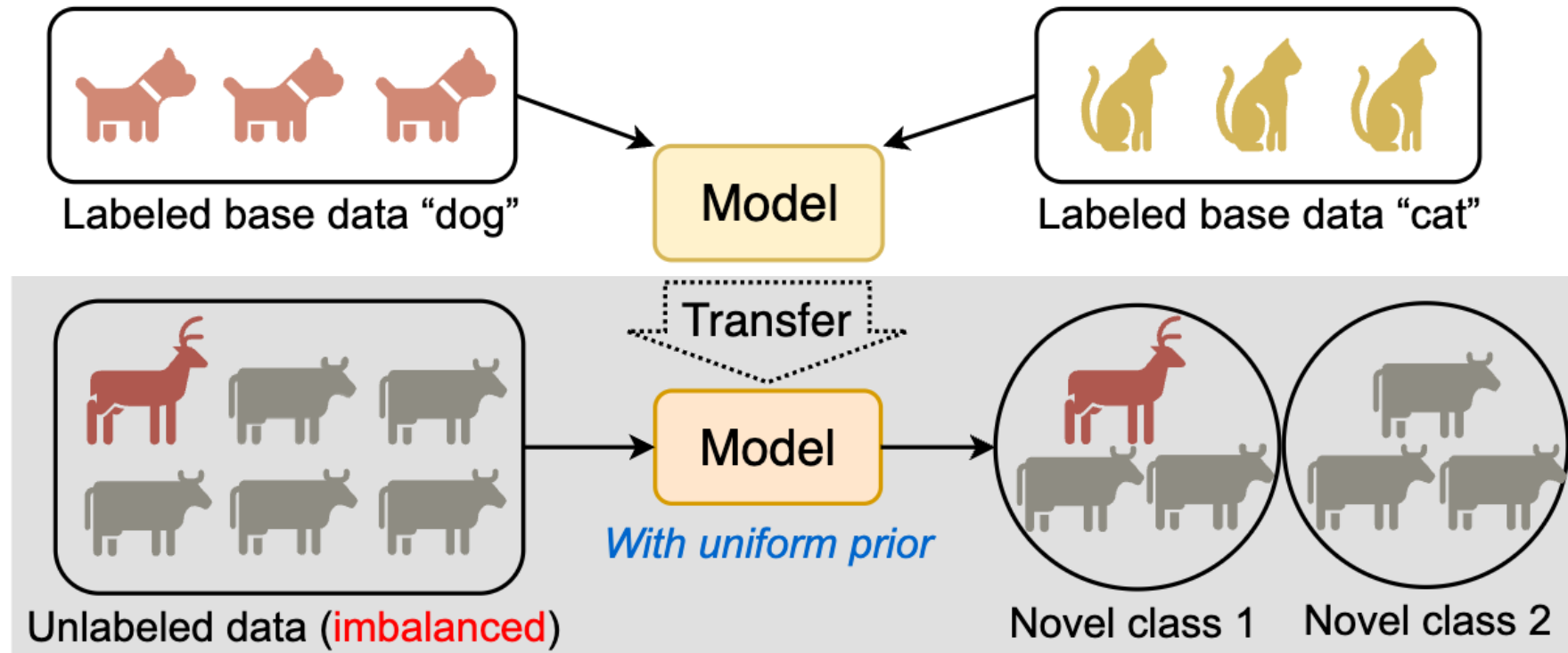


- Existing works often hold a common assumption: unlabeled data has a **uniform class distribution**. But **why?**



- ✓ When ambiguity presents, one can rely on the **uniform clustering prior** according to the uniform class distribution assumption

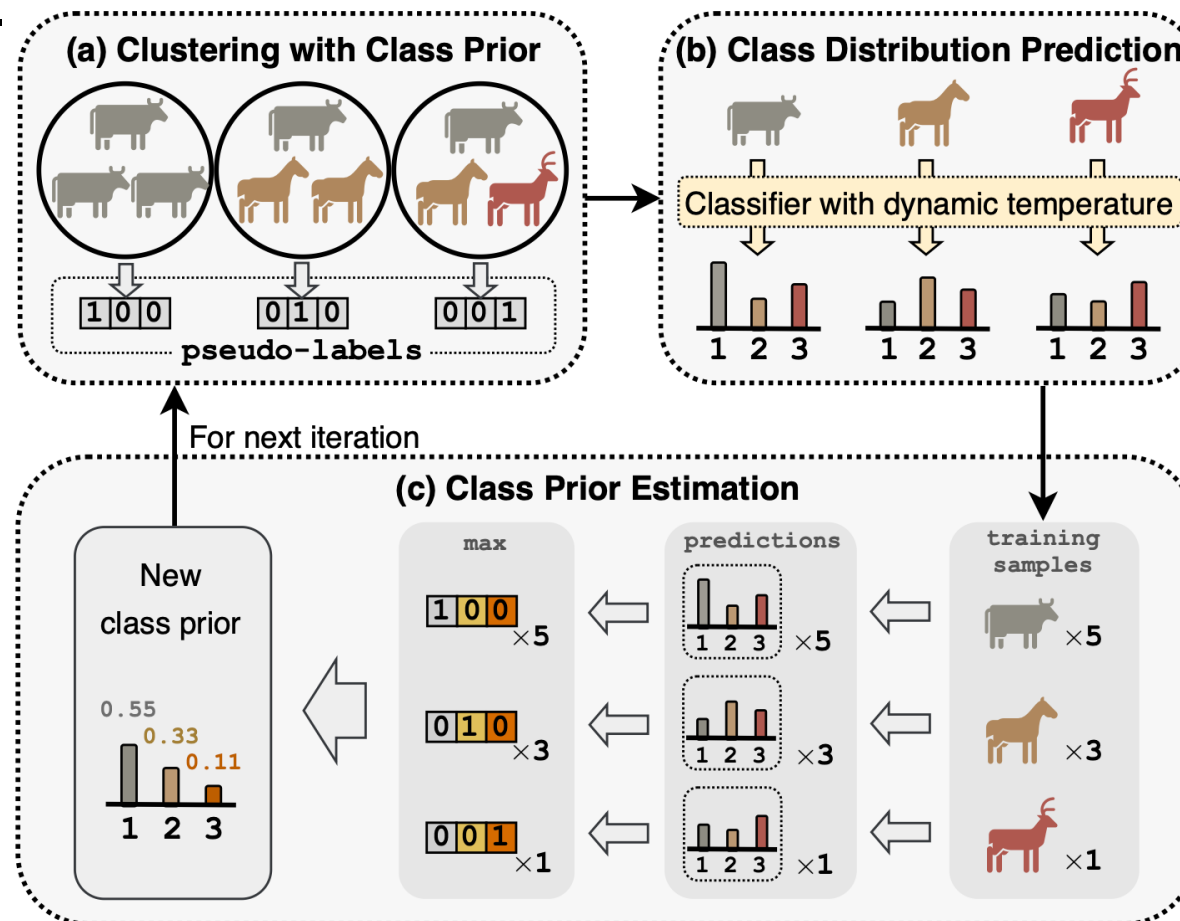
□ However, unlabeled data can hardly be balanced in the real world.



- A chicken-egg problem: prior is necessary, but is unknown (**Distribution-agnostic NCD**)

Approach: overview

- We propose *Bootstrap Your Own Prior (BYOP)* for distribution-agnostic NCD, *i.e.*, to iteratively estimate the class distribution prior using the model prediction itself.



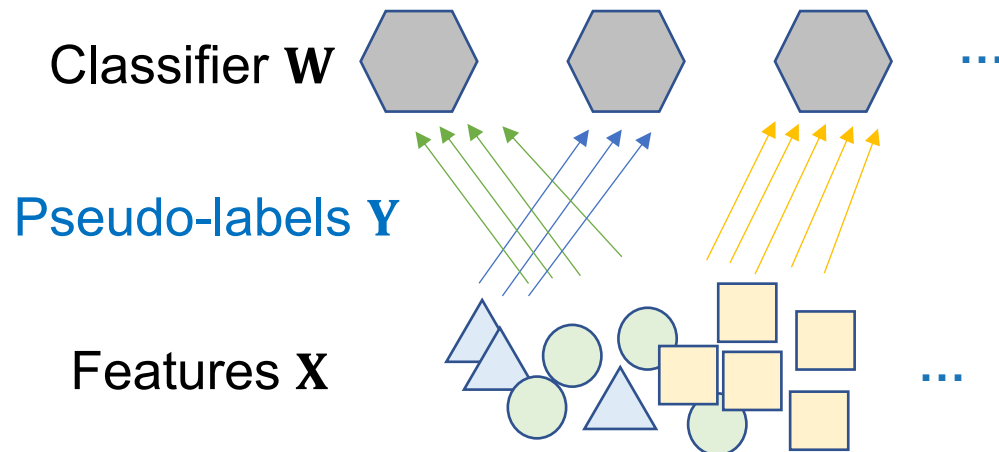
Approach: (1) clustering with class prior

□ Clustering the unlabeled data using the current class prior

Clustering: assigning image features \mathbf{X} to classifier weights \mathbf{W}



An optimal transport (OT) problem



↓ C^n : # of novel classes; B : # of novel samples in a batch

\mathbf{Y} is optimized by

$$\max_{\mathbf{Y} \in \mathcal{T}} \text{tr}(\mathbf{Y}^\top \mathbf{W}^\top \mathbf{X})$$

$$\mathcal{T} = \left\{ \mathbf{Y} \in \mathbb{R}_+^{C^n \times B} \mid \mathbf{Y} \mathbf{1}_B = \mathbf{p}, \mathbf{Y}^\top \mathbf{1}_{C^n} = \frac{1}{B} \mathbf{1}_B \right\}$$



Current class prior (updated in step (3))

Solved by the Sinkhorn-Knopp algorithm

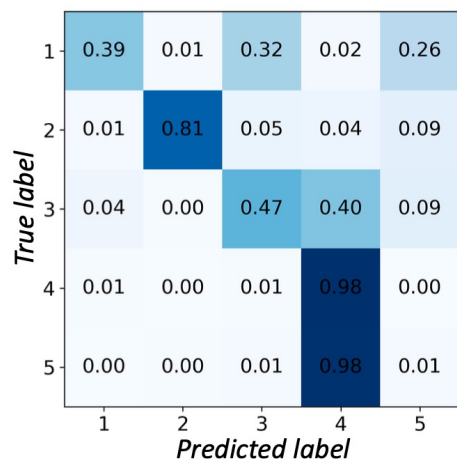
Approach: (2) class distribution prediction

□ Training a classifier using (pseudo-)labels for base/novel data

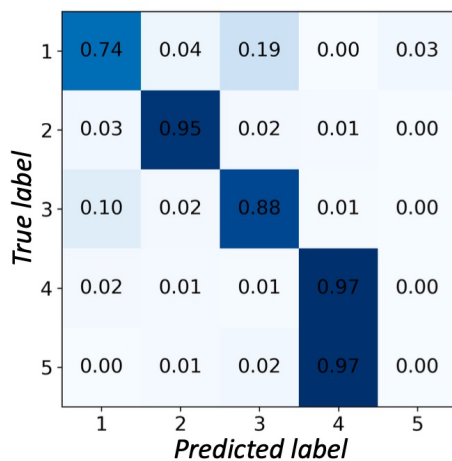
Ambiguity in the pseudo-labels → **ambiguous prediction** for novel samples → inaccurate prior estimation → ...

CE loss: $\mathcal{L}(x, y) = - \sum_{c=1}^C y_c \log(\hat{y}_c)$, $\hat{y} = \underset{\text{softmax}}{\sigma}(q/\tau)$

dynamic temperature: $\tau' = \tau/\rho$, $\rho = \max(\sigma(q/\tau))$



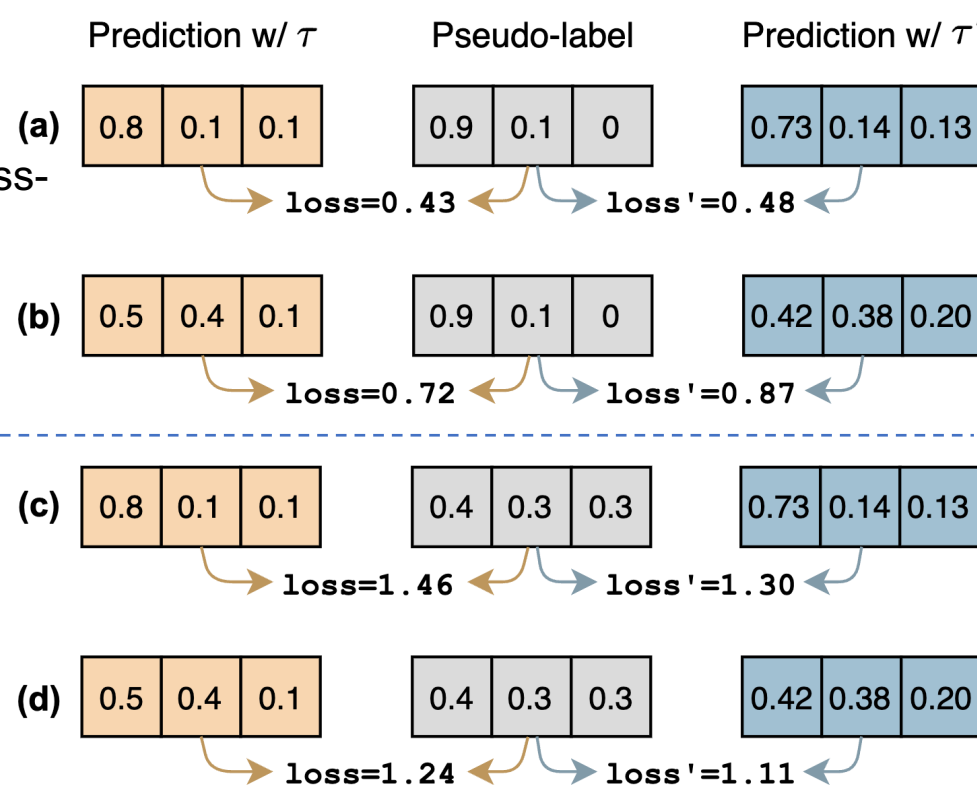
(a) BYOP w/ τ



(b) BYOP w/ τ'

When PL is less-ambiguous: encourage confidence

When PL is ambiguous: preventing learning



Approach: (3) class prior estimation

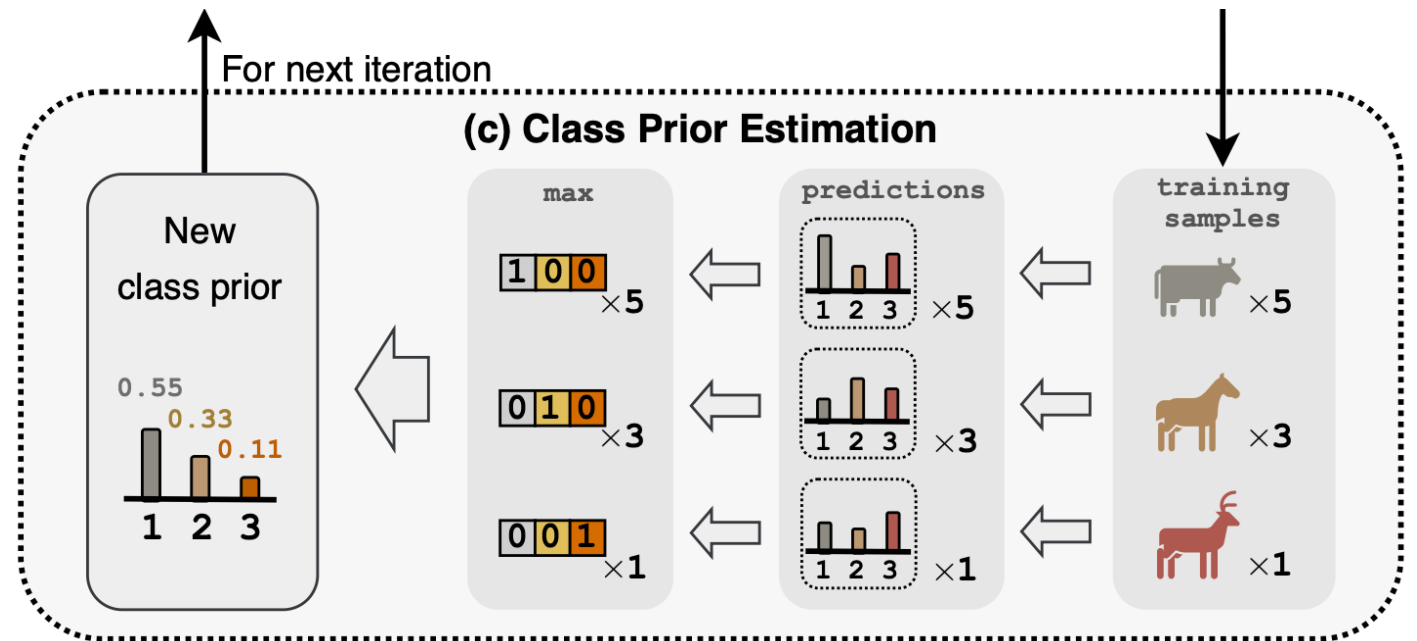
□ Estimating the class prior based on the model prediction

First-in-first-out queue: $\mathcal{K} = \{q_1^u, \dots, q_K^u\}$

$$r_c = \frac{1}{K} \sum_{k=1}^K \mathbb{1}(c = \arg \max_{c' \in S} q_{k,c'}^u)$$
$$S = \{1, \dots, C^u\}$$

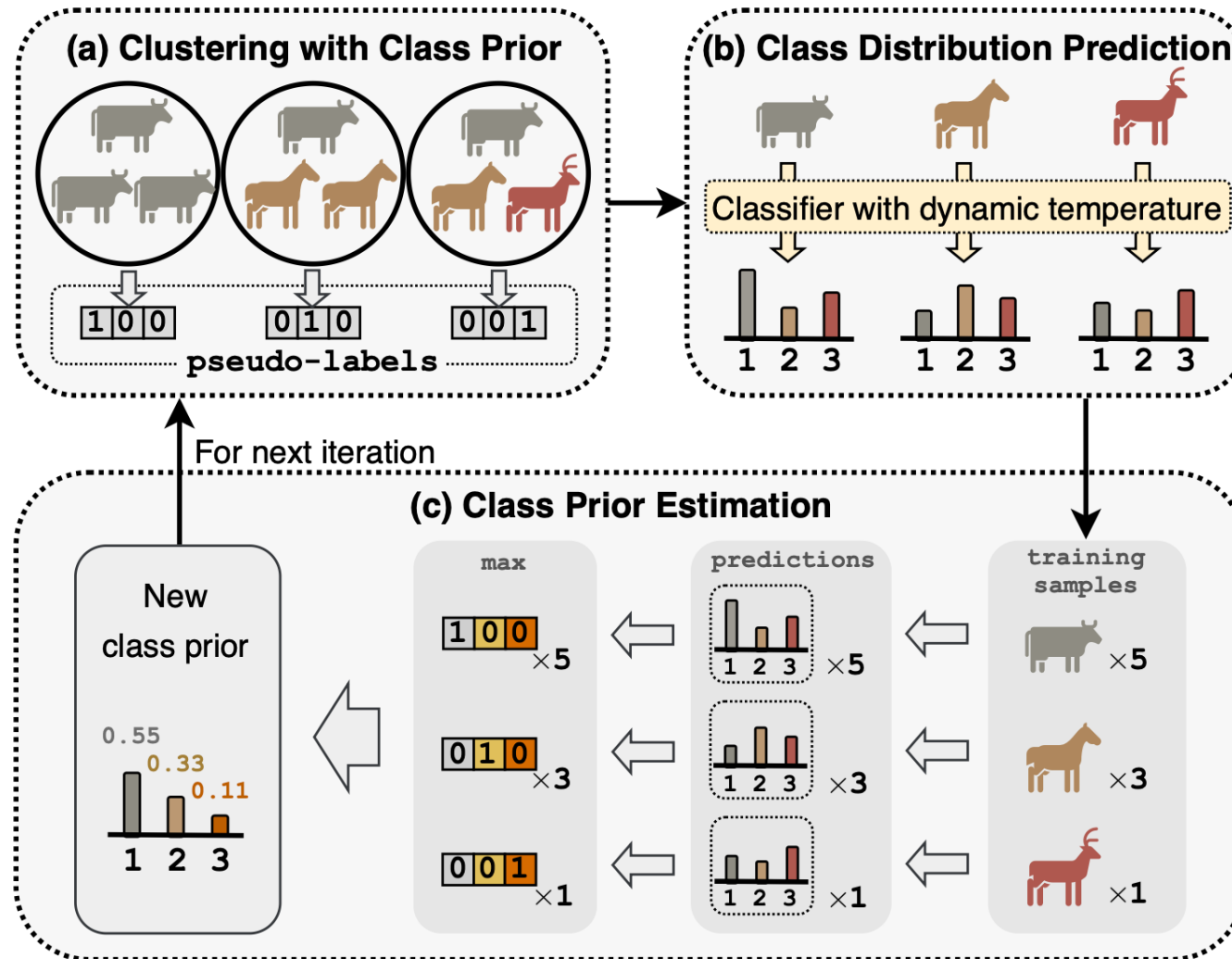
$$\mathbf{p} = \left[\frac{1}{C^u}, \dots, \frac{1}{C^u} \right] \text{ (iteration = 0)}$$

$$\mathbf{p} \leftarrow \mu \mathbf{p} + (1 - \mu) \mathbf{r} \text{ (afterwards)}$$



Approach: overview

□ Bootstrap Your Own Prior (BYOP) for distribution-agnostic NCD



Experiments: datasets

- Each dataset is split into **base subset** and **novel subset**; each subset is again split into **training data** and **testing data**

Subset → Dataset ↓	Base		Novel	
	Images	Classes	Images	Classes
CIFAR10	25K	5	25K	5
CIFAR100-20	40K	80	10K	20
CIFAR100-50	25K	50	25K	50
Tiny-ImageNet	50K	100	50K	100

- For distribution-agnostic NCD, **training data is imbalanced** (controlled by imbalance ratio); **testing data is balanced**

Experiments: evaluation metrics

❑ For distribution-agnostic NCD, training data is imbalanced (controlled by imbalance ratio); testing data is balanced

❑ Metric 1: traditional protocol

➤ Clustering acc on training data of novel subset

❑ Metric 2: task-aware protocol

➤ Classification acc on testing data of base subset

➤ Clustering acc on testing data of novel subset

❑ Metric 3: task-agnostic protocol (Generalized NCD)

➤ Classification/clustering acc on {testing data of base subset, testing data of novel subset}

❑ Clustering acc: $ACC = \frac{1}{M} \sum_{i=1}^M \mathbb{1}[y_i^u = \text{map}(\hat{y}_i^u)]$ (Using Hungarian algorithm)

Experiments: comparison with SOTAs

Dataset →	CIFAR10 (<i>imbalance ratio: 100</i>)							CIFAR10 (<i>imbalance ratio: 10</i>)						
	Trad.	Task-aware			Task-agnostic			Trad.	Task-aware			Task-agnostic		
Protocol →	Nov.	Base	Nov.	All	Base	Nov.	All	Nov.	Base	Nov.	All	Base	Nov.	All
Method ↓	Nov.	Base	Nov.	All	Base	Nov.	All	Nov.	Base	Nov.	All	Base	Nov.	All
RS [12]	46.3	71.8	43.2	57.5	–	–	–	<u>69.7</u>	87.4	<u>63.6</u>	75.5	–	–	–
RS+ [12]	45.3	64.4	50.1	57.3	64.4	55.5	60.0	66.5	77.3	63.3	70.3	77.3	62.3	69.8
NCL [56]	47.2	<u>71.6</u>	43.1	57.4	–	–	–	62.6	86.9	56.9	71.9	–	–	–
UNO [11]	43.9	69.6	52.2	60.9	56.0	55.6	55.8	59.6	88.1	59.1	73.6	78.2	58.8	68.5
UNO + BYOP	59.3	70.1	53.3	61.7	56.6	56.6	56.6	63.2	<u>88.5</u>	61.7	75.1	78.4	61.0	69.7
ComEx [47]	44.6	70.0	<u>53.8</u>	<u>61.9</u>	57.8	55.1	56.5	68.1	87.9	63.5	<u>75.7</u>	<u>81.3</u>	<u>63.3</u>	<u>72.3</u>
ComEx + BYOP	<u>57.0</u>	71.4	54.5	63.0	<u>59.3</u>	<u>56.0</u>	<u>57.7</u>	72.1	88.7	65.5	77.1	82.2	65.4	73.8

Dataset →	CIFAR100-50 (<i>imbalance ratio: 100</i>)							CIFAR100-50 (<i>imbalance ratio: 10</i>)						
	Trad.	Task-aware			Task-agnostic			Trad.	Task-aware			Task-agnostic		
Protocol →	Nov.	Base	Nov.	All	Base	Nov.	All	Nov.	Base	Nov.	All	Base	Nov.	All
Method ↓	Nov.	Base	Nov.	All	Base	Nov.	All	Nov.	Base	Nov.	All	Base	Nov.	All
RS [12]	30.7	40.8	23.3	32.1	–	–	–	27.4	48.4	23.7	36.1	–	–	–
RS+ [12]	29.6	35.5	23.0	29.3	35.5	22.5	29.0	26.0	38.5	23.4	31.0	38.5	21.9	30.2
NCL [56]	30.4	39.9	21.8	30.9	–	–	–	27.8	47.0	23.4	35.2	–	–	–
UNO [11]	25.7	44.8	21.3	33.1	36.9	22.6	29.8	33.7	63.9	32.5	48.2	53.6	30.8	42.2
UNO + BYOP	35.5	45.4	<u>23.4</u>	<u>34.4</u>	37.3	<u>24.0</u>	30.7	38.3	<u>64.6</u>	34.9	49.8	54.1	33.0	43.6
ComEx [47]	27.1	<u>45.9</u>	22.6	34.3	<u>39.5</u>	23.3	<u>31.4</u>	34.3	64.6	32.6	48.6	<u>57.7</u>	31.9	44.8
ComEx + BYOP	<u>33.1</u>	46.9	24.1	35.5	40.9	24.4	32.7	<u>37.4</u>	65.3	<u>33.5</u>	<u>49.4</u>	58.5	<u>32.8</u>	45.7

□ + Logit Adjustment* (post-hoc adjustment using estimated prior)

CIFAR100-50 with imbalance ratio 100 (task-aware)

Subset →	Base (<i>test</i>)				Novel (<i>test</i>)			
	Many	Med.	Few	All	Many	Med.	Few	All
Method ↓								
UNO [11]	78.5	41.9	14.1	44.8	23.8	24.7	15.4	21.3
UNO + BYOP	76.6	44.2	15.4	45.4	33.6	24.1	12.4	23.4
UNO + BYOP [†]	76.3	47.9	18.9	47.7	28.6	30.2	12.9	23.8

$$q^\dagger = q - \tau \log(p)$$

*Long-Tail Learning via Logit Adjustment, ICLR'21

Experiments: ablation study

□ Estimated prior p , dynamic temperature τ

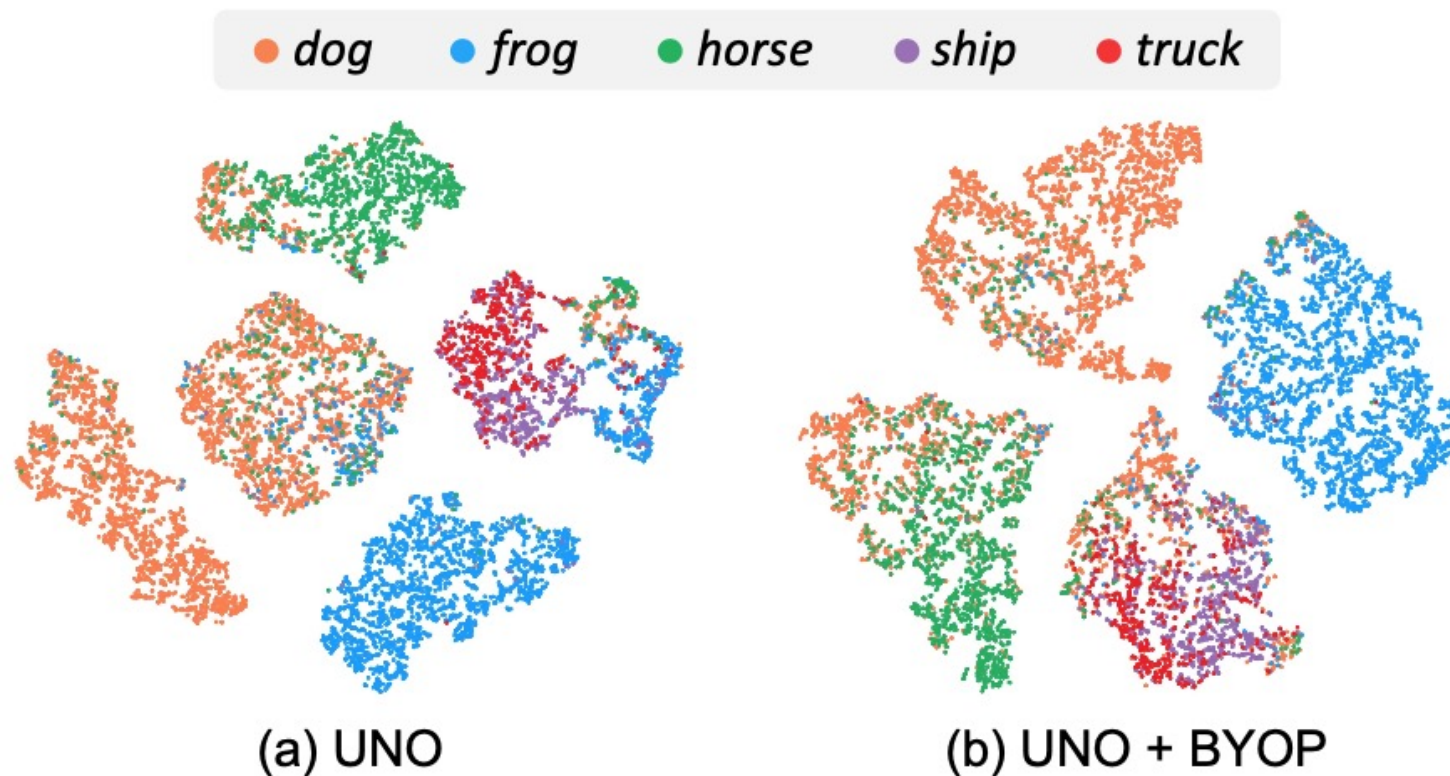
CIFAR100-50 with imbalance ratio 100 (traditional, task-aware)

Subset (<i>split</i>) →	Novel (<i>training</i>)				Base (<i>test</i>)				Novel (<i>test</i>)			
	Many	Med.	Few	All	Many	Med.	Few	All	Many	Med.	Few	All
Uniform p	24.6	33.9	16.1	25.7	78.5	41.9	14.1	44.8	23.8	24.7	15.4	21.3
Oracle p	32.1	28.1	12.0	30.8	77.4	43.4	15.1	45.3	27.2	28.3	12.9	22.8
Estimated p	29.7	31.0	14.6	29.4	76.1	43.4	15.2	44.9	28.7	23.4	15.6	22.6
Uniform p + dynamic τ	26.8	33.6	15.7	27.5	76.5	43.7	15.4	45.2	27.0	27.8	12.5	22.4
Oracle p + dynamic τ	39.1	28.7	11.0	36.5	76.6	43.6	16.6	45.6	36.0	22.7	11.0	23.2
Estimated p + dynamic τ	37.7	28.6	13.9	35.5	76.6	44.2	15.4	45.4	33.6	24.1	12.4	23.4

Experiments: visualization

□ t-SNE visualizations of the 5 novel classes (training data of CIFAR10)

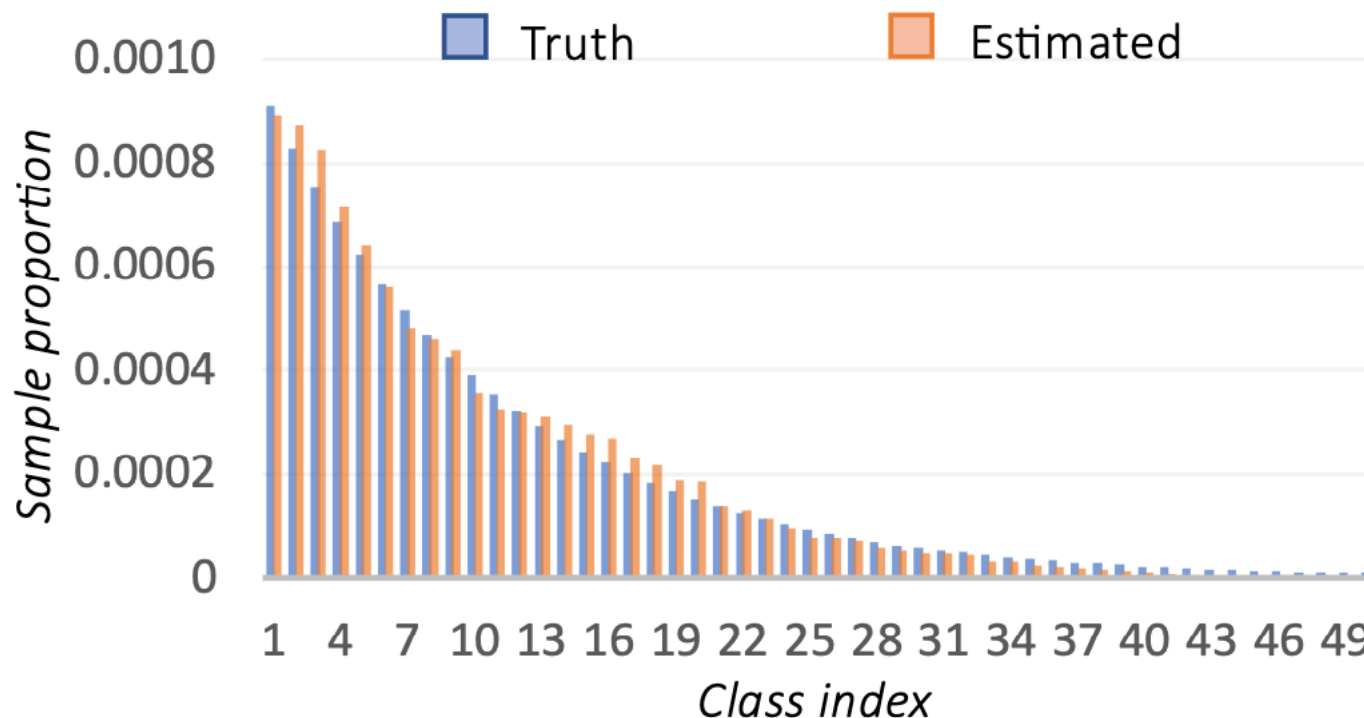
imbalance ratio: 10



Experiments: visualization

Estimated prior vs. true prior

CIFAR100-50 with imbalance ratio 100



Code: <https://github.com/muliyangm/BYOP>

Thank you for listening!