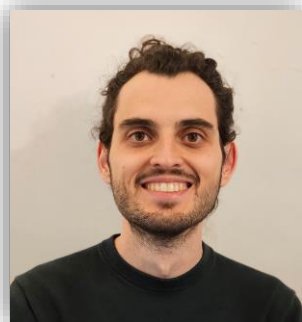


# Conformal Prediction for Zero-Shot Models

Julio  
Silva-Rodríguez



Ismail  
Ben Ayed

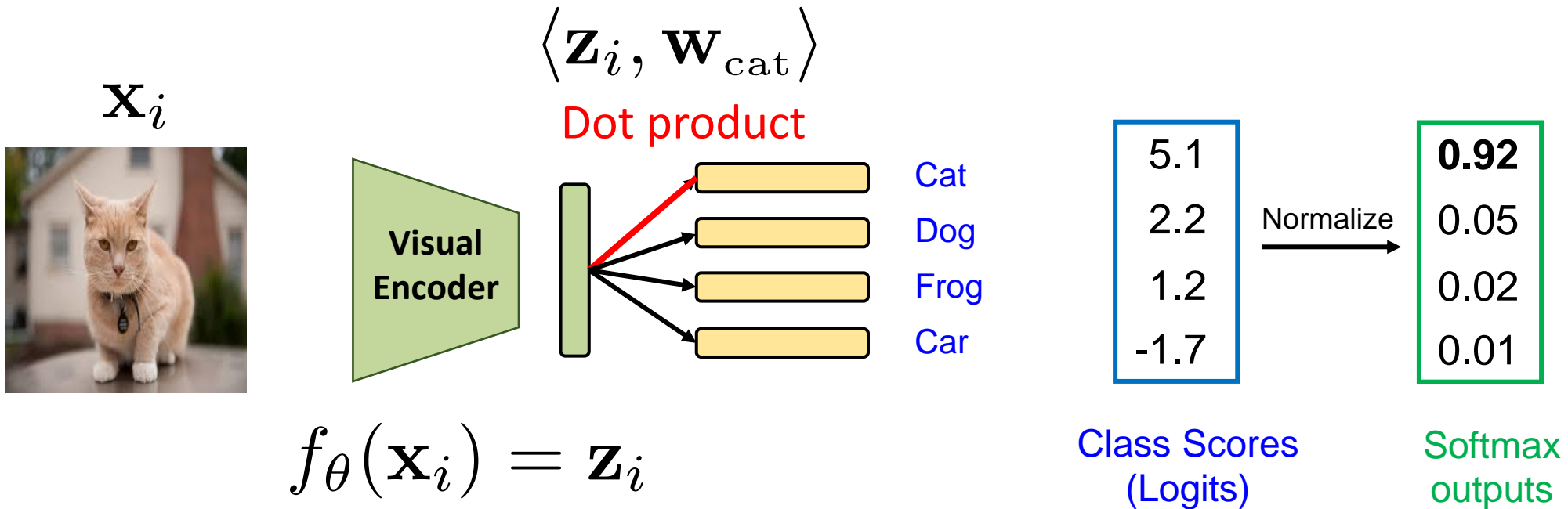


Jose Dolz

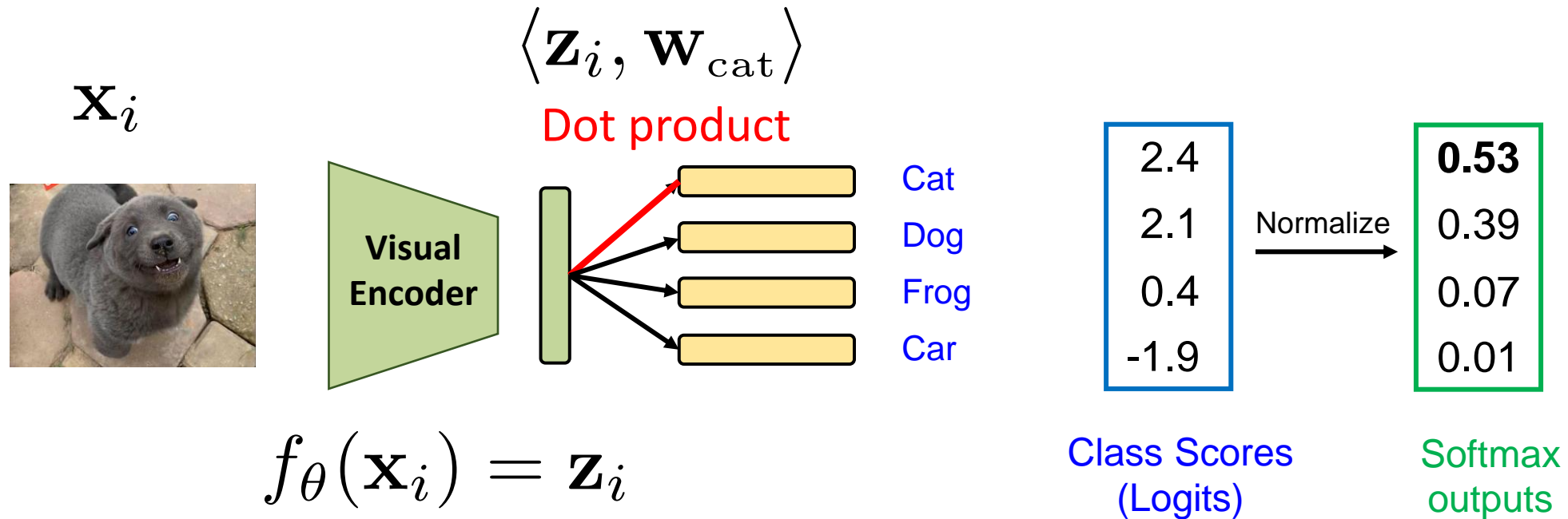


ÉTS Montréal

# Reliability and uncertainty on vision classifiers



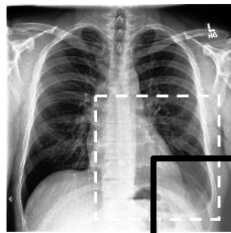
# Reliability and uncertainty on vision classifiers



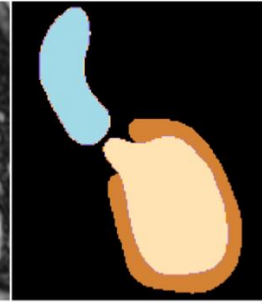
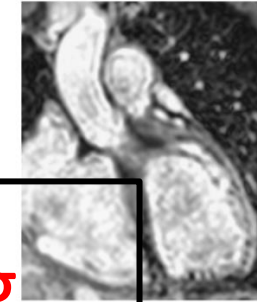
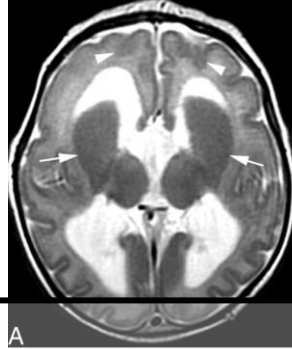
# Reliability and uncertainty on vision classifiers



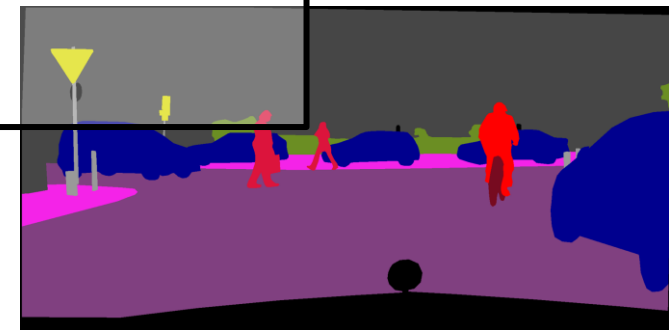
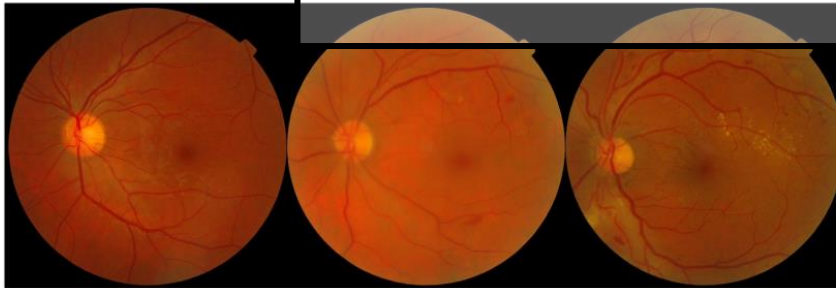
Severe **cardiomegaly** is noted in the image with enlarged...



Radiograph shows **pleural effusion** in the right lobe...

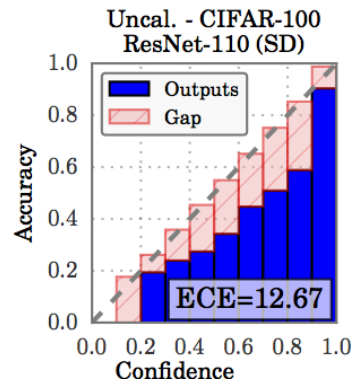
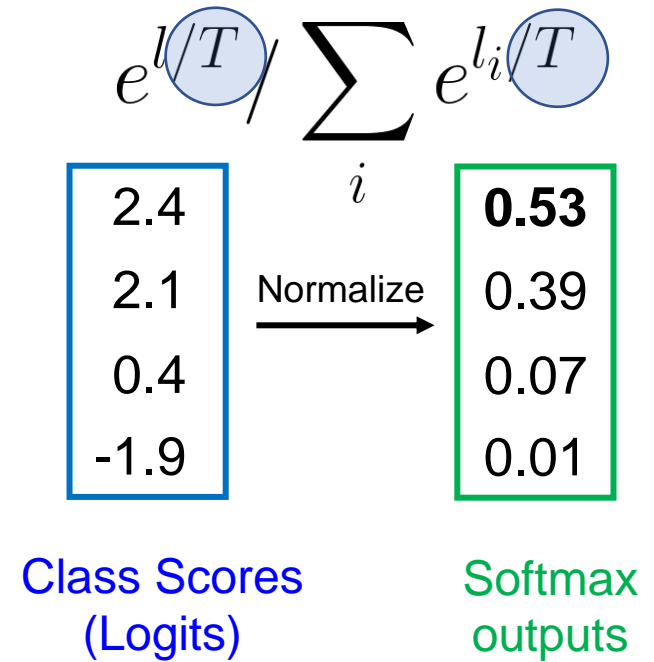
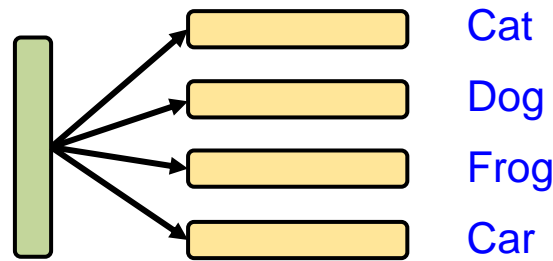
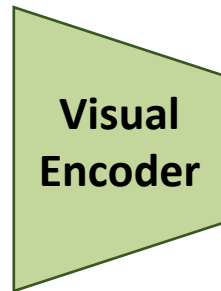


Vision classifiers are being  
deployed at high-stake  
applications!



# Reliability and uncertainty on vision classifiers

## ■ Model calibration

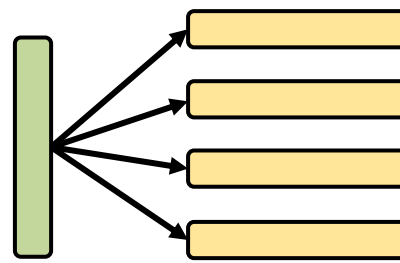


# Reliability and uncertainty on vision classifiers

## ■ Model calibration



Visual  
Encoder

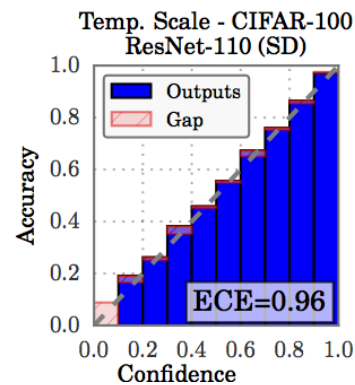
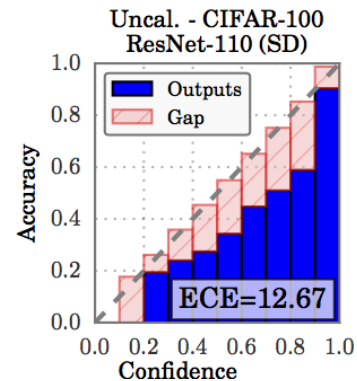


Cat

Dog

Frog

Car



validation data

$$\frac{e^{l_i/T}}{\sum_i e^{l_i/T}}$$

2.4

2.1

0.4

-1.9

Normalize

**0.53**

0.39

0.07

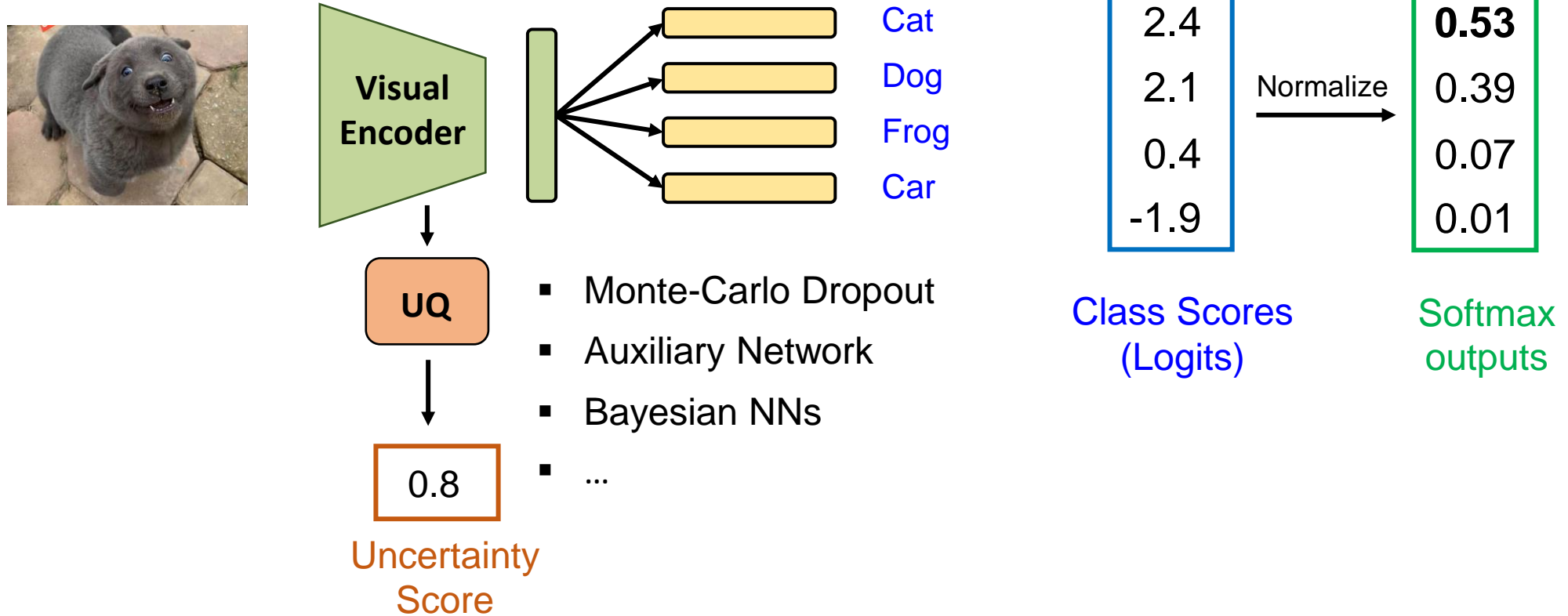
0.01

Class Scores  
(Logits)

Softmax  
outputs

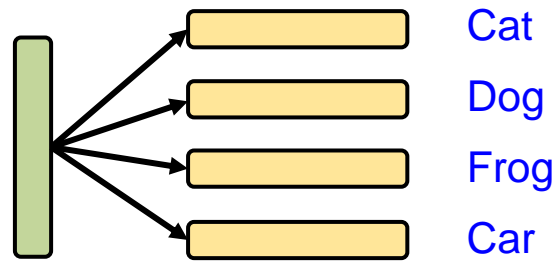
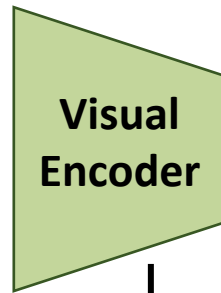
# Reliability and uncertainty on vision classifiers

## ■ Uncertainty quantification



# Reliability and uncertainty on vision classifiers

## ■ Uncertainty quantification



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2.1  
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-1.9

Class Scores  
(Logits)

Normalize

**0.53**  
0.39  
0.07  
0.01

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outputs

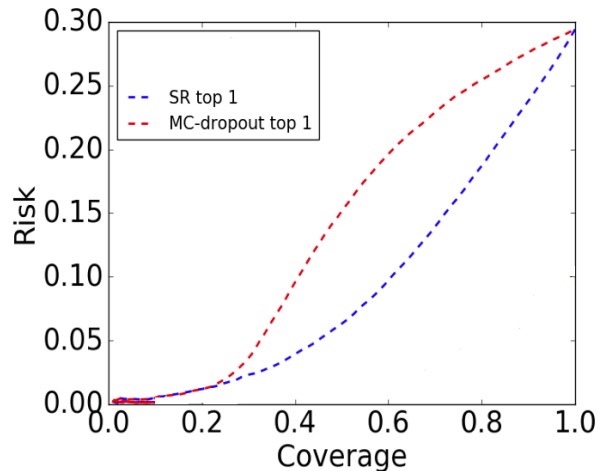
uq

- Monte-Carlo Dropout
- Auxiliary Network
- Bayesian NNs
- ...

0.8

Uncertainty  
Score

### Rejection Criteria



Plot modified from [Geifman et al., Selective Classification for Deep Neural Networks, NIPS 2017]



# Reliability and uncertainty on vision classifiers

- Limitations, pitfalls.

## 1. Why to reject samples?



Cat ( $p=0.53$ ,  $u=0.8$ )  
REJECT **X**



{Cat ( $p=0.53$ ),  
**Dog** ( $p=0.29$ )}

# Reliability and uncertainty on vision classifiers

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{Cat ( $p=0.53$ ),  
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Weight	Acc@1	Acc@5
AlexNet_Weights.IMAGENET1K_V1	56.522	79.066
ConvNeXt_Base_Weights.IMAGENET1K_V1	84.062	96.87
ConvNeXt_Large_Weights.IMAGENET1K_V1	84.414	96.976
ConvNeXt_Small_Weights.IMAGENET1K_V1	83.616	96.65
ConvNeXt_Tiny_Weights.IMAGENET1K_V1	82.52	96.146
DenseNet121_Weights.IMAGENET1K_V1	74.434	91.972
DenseNet161_Weights.IMAGENET1K_V1	77.138	93.56
DenseNet169_Weights.IMAGENET1K_V1	75.6	92.806
DenseNet201_Weights.IMAGENET1K_V1	76.896	93.37
EfficientNet_B0_Weights.IMAGENET1K_V1	77.692	93.532
EfficientNet_B1_Weights.IMAGENET1K_V1	78.642	94.186

<https://pytorch.org/vision/stable/models.html>



{**fox squirrel**}



{marmot, **fox squirrel**,  
mink, weasel, beaver}

From [Uncertainty Sets for Image Classifiers Using Conformal Prediction, ICLR 2021]

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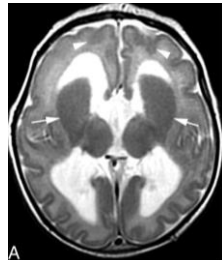
{**fox squirrel**}



{marmot, **fox squirrel**,  
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From [Uncertainty Sets for Image Classifiers Using Conformal Prediction, ICLR 2021]

### 2. Lack of *guarantees*.



*“Set of predictions that covers the true diagnosis with a high probability (e.g., 95%)”.*

# (Brief) Introduction to (split) Conformal Prediction

*Conformal prediction (CP) is a machine learning framework that provides **model agnostic**, and **distribution-free**, **finite-sample validity guarantees** for handling reliability, by producing **predictive sets**.*

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- Random data points  $(\mathbf{x}, y)$  from a data distribution  $\mathcal{P}_{\mathcal{X}\mathcal{Y}}$ .
- Label space  $\mathcal{Y} = \{1, 2, \dots, K\}$ .
- Set-valued mapping function  $\mathcal{C} : \mathcal{X} \rightarrow 2^K$ , such that  $C(\mathbf{x}) \subset \mathcal{Y}$ .
- Desired error level  $\alpha \in (0, 1)$ .

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***Coverage property***

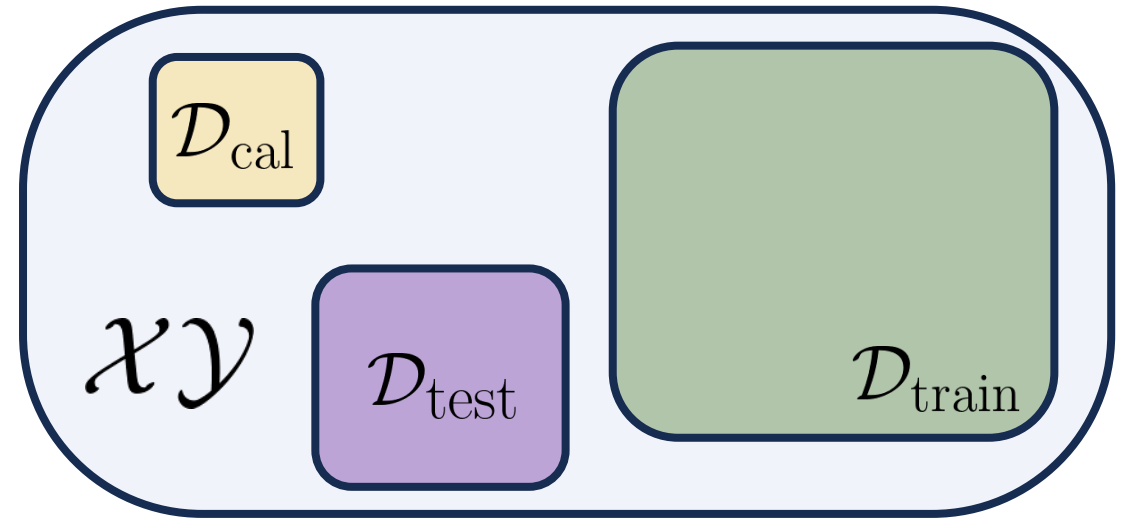
$$\mathcal{P}(Y \in C(\mathbf{x})) \geq 1 - \alpha$$

(marginal over  $\mathcal{P}_{\mathcal{X}\mathcal{Y}}$ )

# (Brief) Introduction to (split) Conformal Prediction

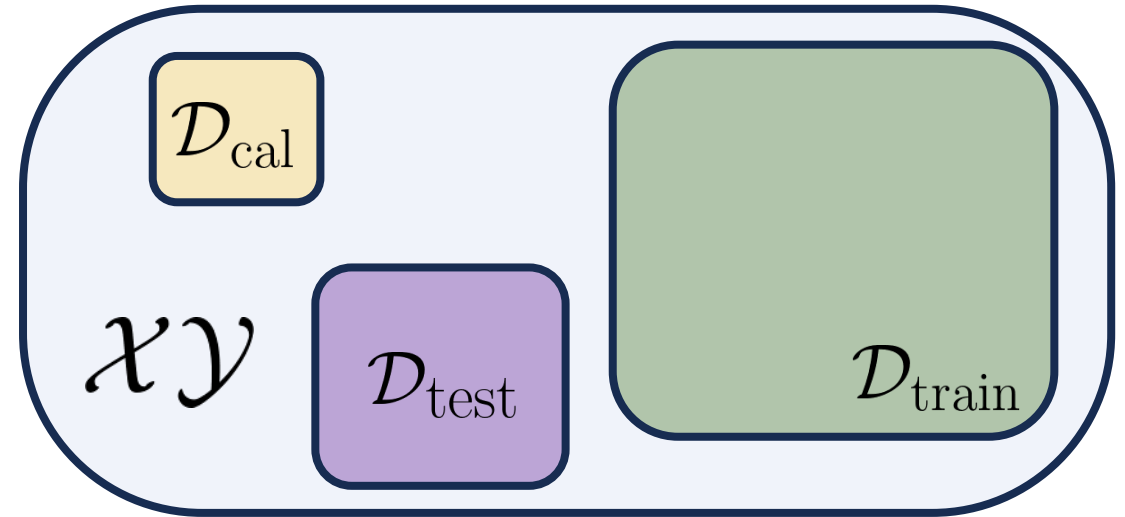
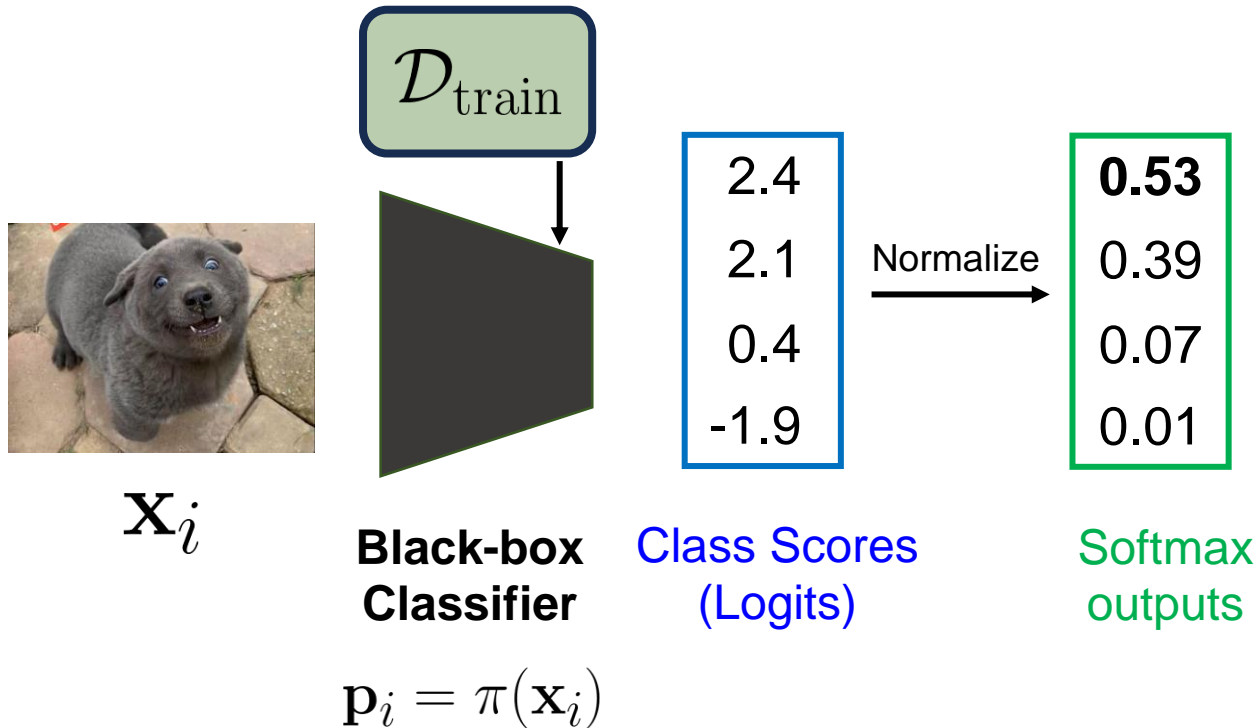
Setting

- **Split conformal prediction (SCP).**



# (Brief) Introduction to (split) Conformal Prediction

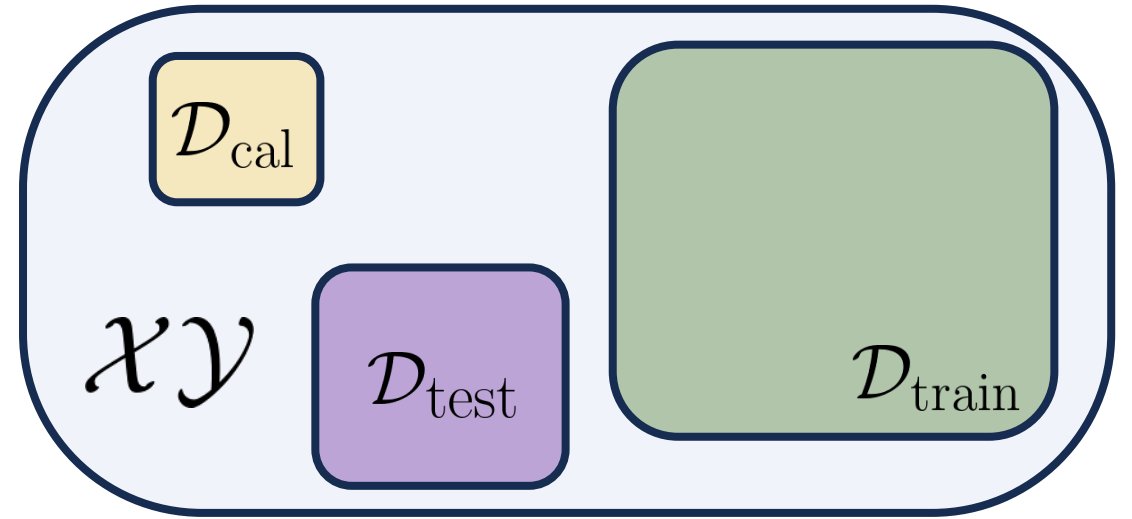
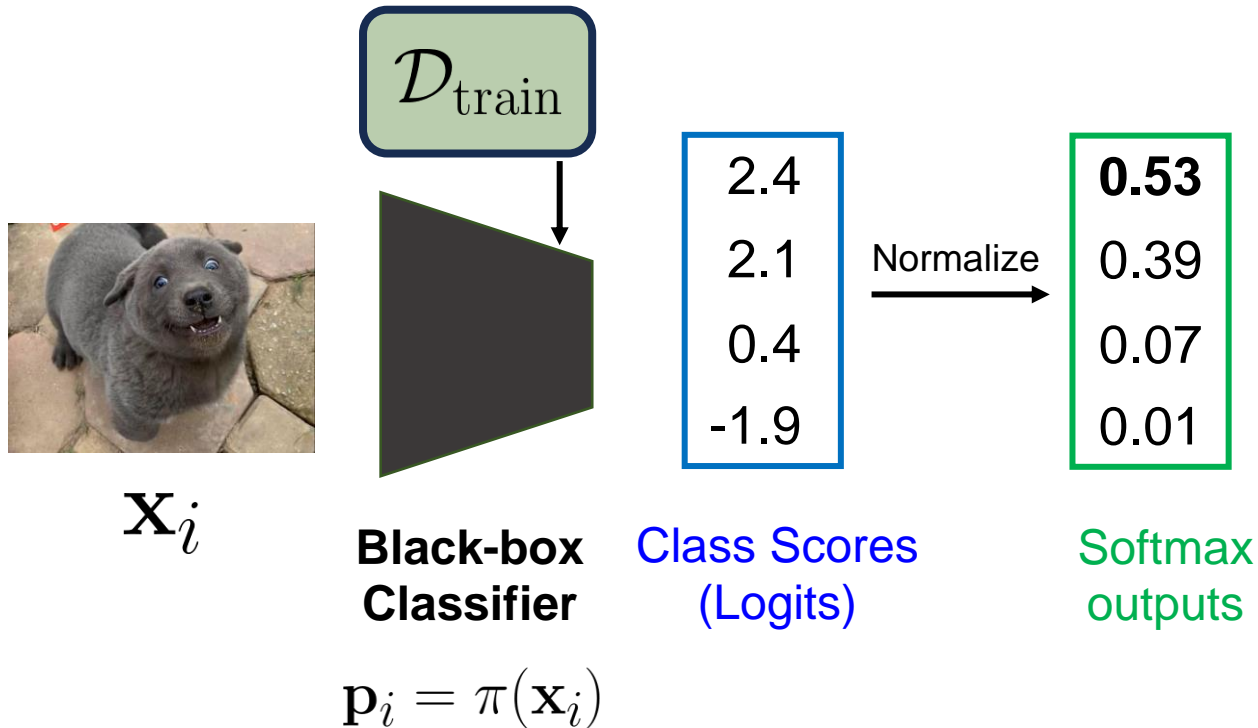
## ▪ Split conformal prediction (SCP).





# (Brief) Introduction to (split) Conformal Prediction

## Split conformal prediction (SCP).



$$\mathcal{D}_{\text{cal}} = \{(\pi(\mathbf{x}_i), y_i)\}_{i=1}^N$$

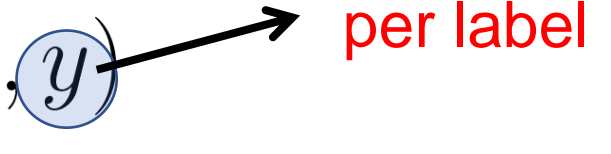
$$\mathcal{D}_{\text{test}} = \{(\pi(\mathbf{x}_i), )\}_{i=N+1}^{N+M}$$

# (Brief) Introduction to (split) Conformal Prediction

## ▪ Split conformal prediction (SCP).

1. Define a non-conformity score.

$$s_{(y)} = \mathcal{S}(\mathbf{p}, y)$$

evaluated  
per label

0.53	0.47
0.39	0.61
0.07	0.93
0.01	0.99

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LAC

2. Compute the cumulative score distribution from the calibration set for true labels.

$$s_i = \mathcal{S}(\mathbf{p}_i, y_i)$$

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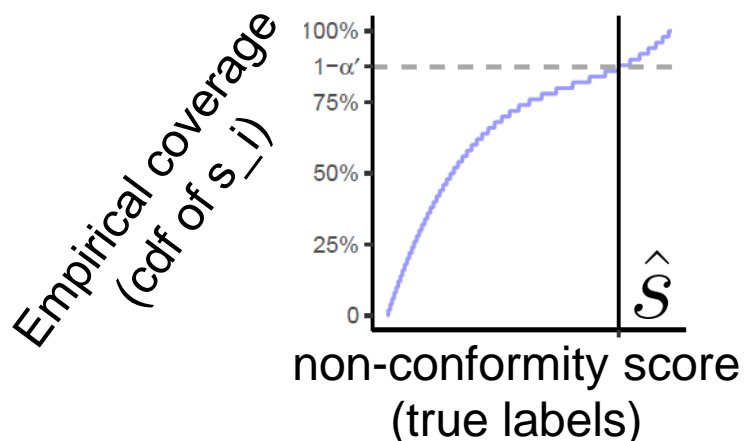
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3. Search the 1-alpha quantile in such distribution.

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$\mathcal{D}_{\text{cal}}$

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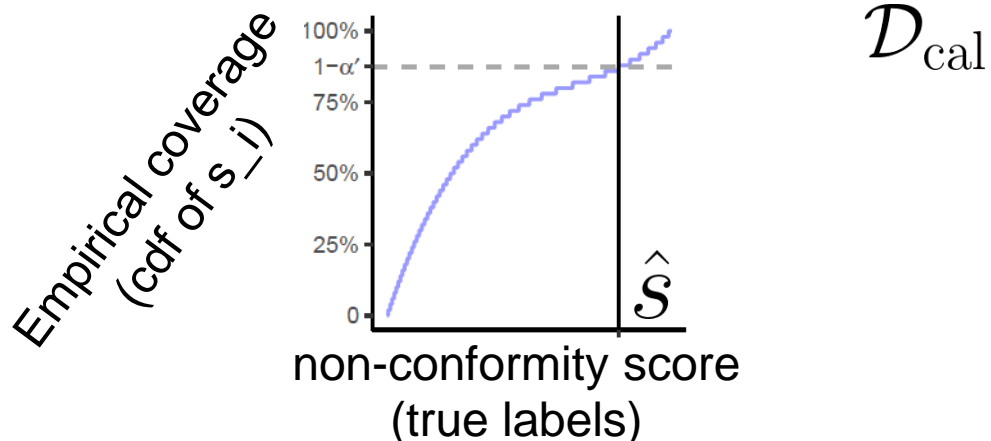
LAC

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3. Search the 1-alpha quantile in such distribution.

$$s_i = \mathcal{S}(\mathbf{p}_i, y_i)$$

0.61



4. Produce output sets for new data points.

$$\mathcal{C}(\mathbf{x}) = \{y \in \mathcal{Y} : \mathcal{S}(\mathbf{p}, y) \leq \hat{s}\}$$

# (Brief) Introduction to (split) Conformal Prediction

## ▪ Split conformal prediction (SCP).

### Theoretical guarantees

$$\mathcal{P}(Y \in C(\mathbf{x})) \geq 1 - \alpha$$

*Generally, there exist theoretical finite-sample coverage guarantees under the assumption of **i.i.d** or, at least, **exchangeable** data distributions for calibration and testing.*

$\mathcal{D}_{\text{cal}}$        $\mathcal{D}_{\text{test}}$   
    ↘      ↙  
    **same marginals!**

# (Brief) Introduction to (split) Conformal Prediction

## ▪ Split conformal prediction (SCP).

### 1. Efficiency

(we want small sets)

$$\text{Size}(\mathcal{D}) = \frac{1}{I} \sum_{i \in \mathcal{D}} |C(\mathbf{x}_i)|$$

### 2. Empirical Coverage

(keep the desired error)

$$\text{Cov}(\mathcal{D}) = \frac{1}{I} \sum_{i \in \mathcal{D}} \delta[(y_i \in C(\mathbf{x}_i))]$$

### 3. Adaptability

(set size should adapt to give coverage to difficult subgroups)

$$\text{CCV}(\mathcal{D}) = 100 \times \frac{1}{|\mathcal{Y}|} \sum_{k \in \mathcal{Y}} |\text{Cov}(\mathcal{D}_k) - (1 - \alpha)|$$



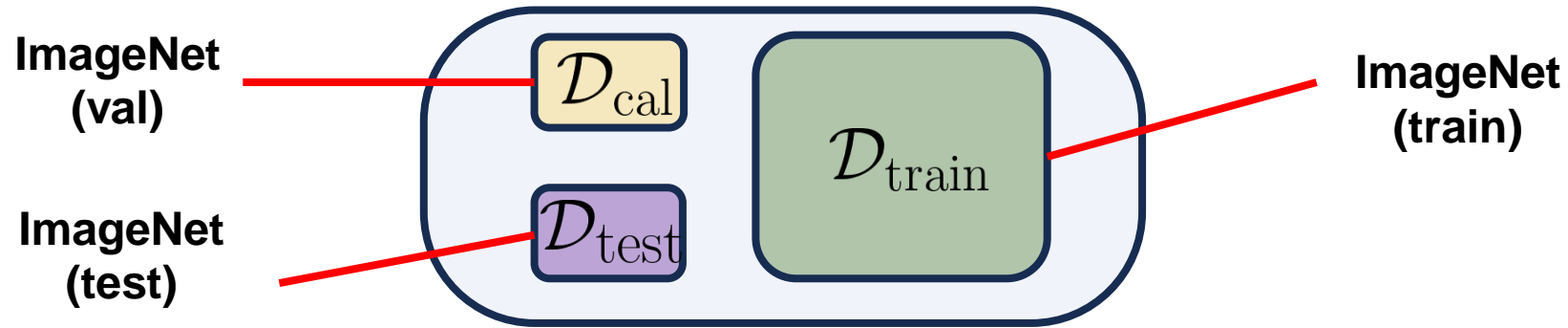
{**fox squirrel**}



{marmot, **fox squirrel**,  
mink, weasel, beaver}

# Literature in Vision Classifiers

- Explored in the standard supervised scenario.



- Different adaptive non-conformity scores have been proposed.

$$\mathcal{S}_{\text{LAC}}(\mathbf{x}, y) = 1 - p_{k=y}$$

[Sadinle et al., Least ambiguous set-valued classifiers with bounded error levels, Jour. American Statistical Association 2019]

$$\mathcal{S}_{\text{APS}}(\mathbf{x}, y) = \rho_x(y) + p_{k=y} \cdot u$$

[Romano et al., Classification with valid and adaptive coverage., NeurIPS 2020]

$$\mathcal{S}_{\text{RAPS}}(\mathbf{x}, y) = \mathcal{S}_{\text{APS}}(\mathbf{x}, y) + \lambda \cdot (o(\mathbf{x}, y) - k_{\text{reg}})^+$$

[Angelopoulos et al., Uncertainty Sets for Image Classifiers Using Conformal Prediction, ICLR 2021]

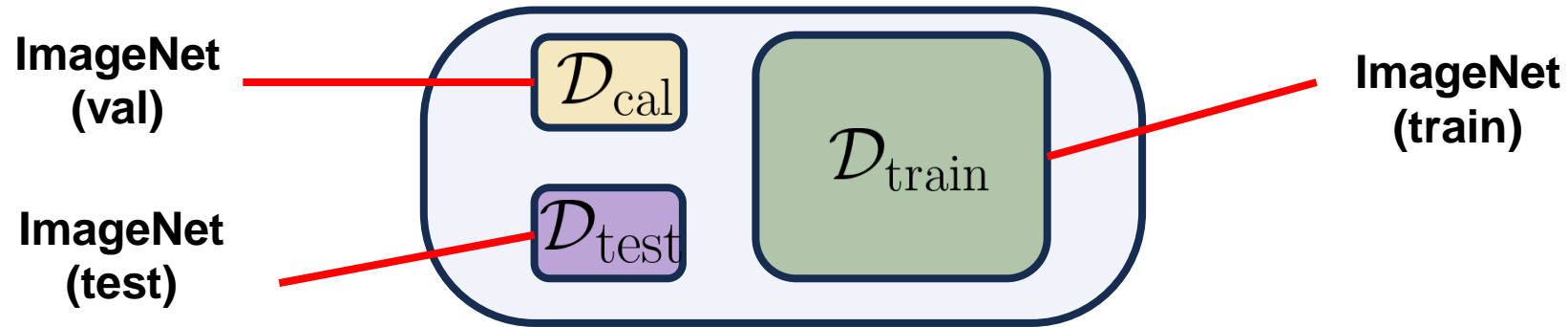


# Literature in Vision Classifiers

Not yet explored  
for vision-language (CLIP)  
models



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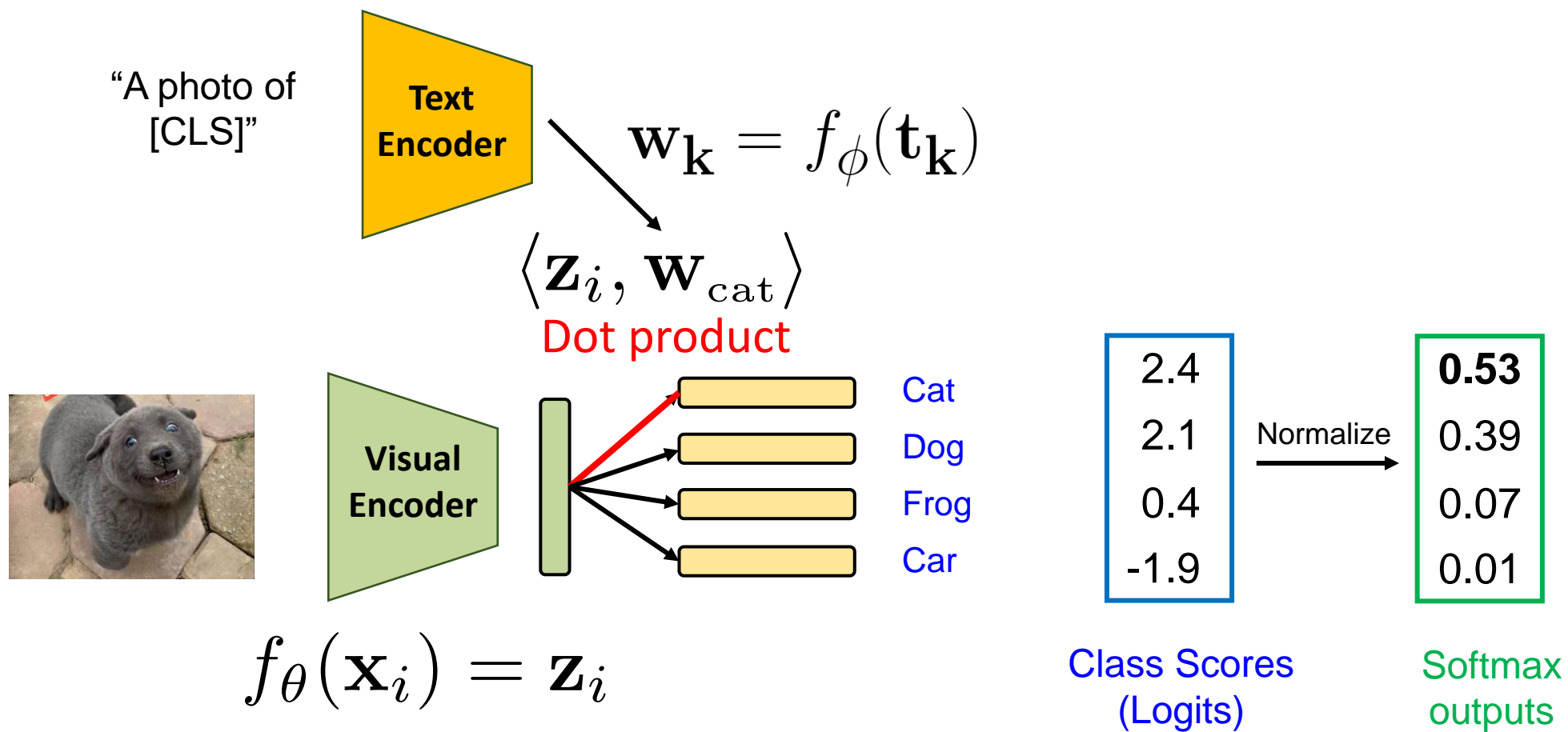
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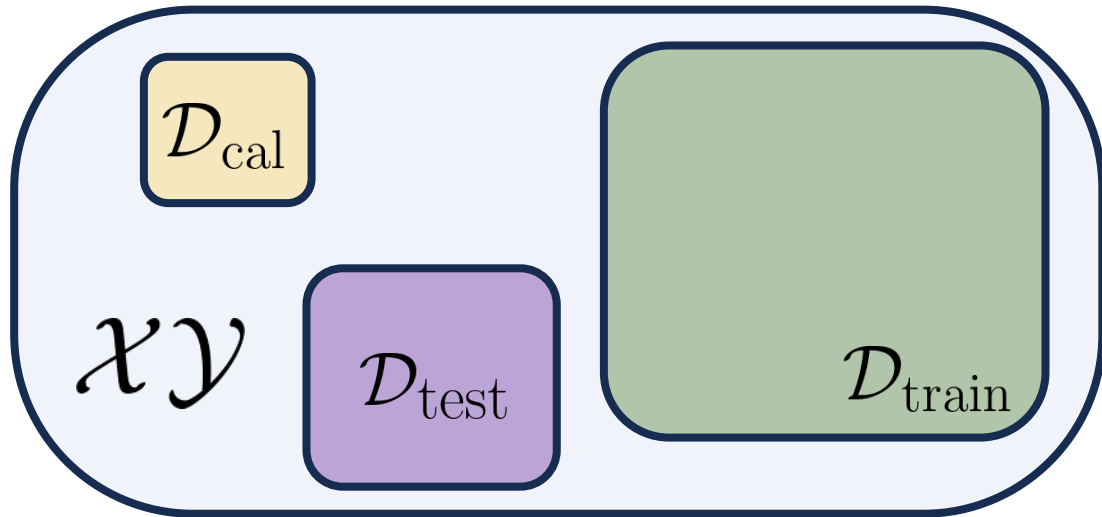
[Angelopoulos et al., Uncertainty Sets for Image Classifiers Using Conformal Prediction, ICLR 2021]

# Vision-Language (zero-shot) Models

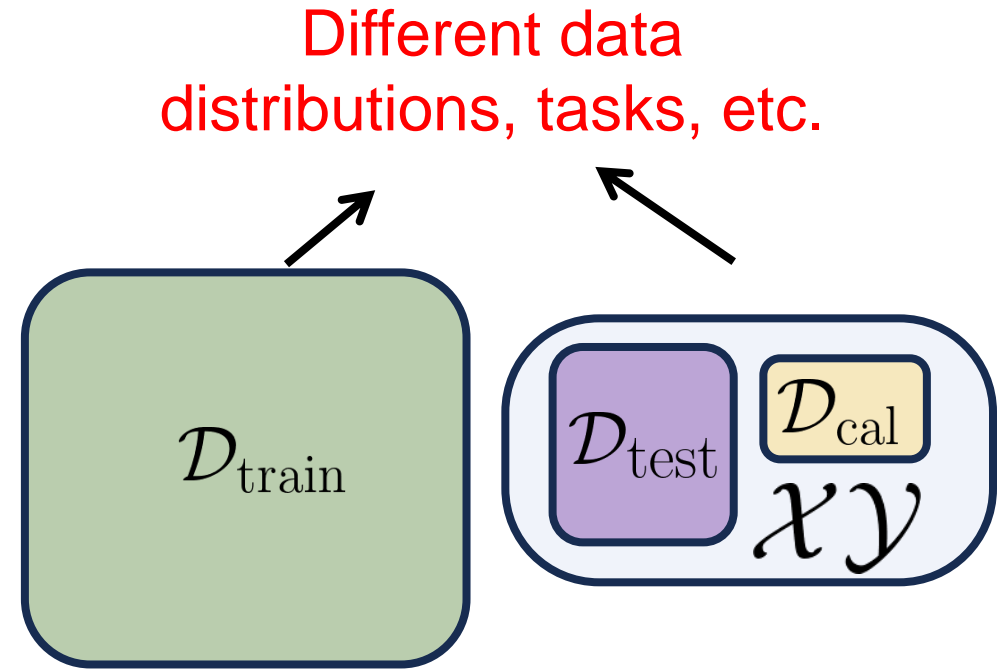


# Conformal Prediction for Zero-Shot Models

- Transfer learning setting.



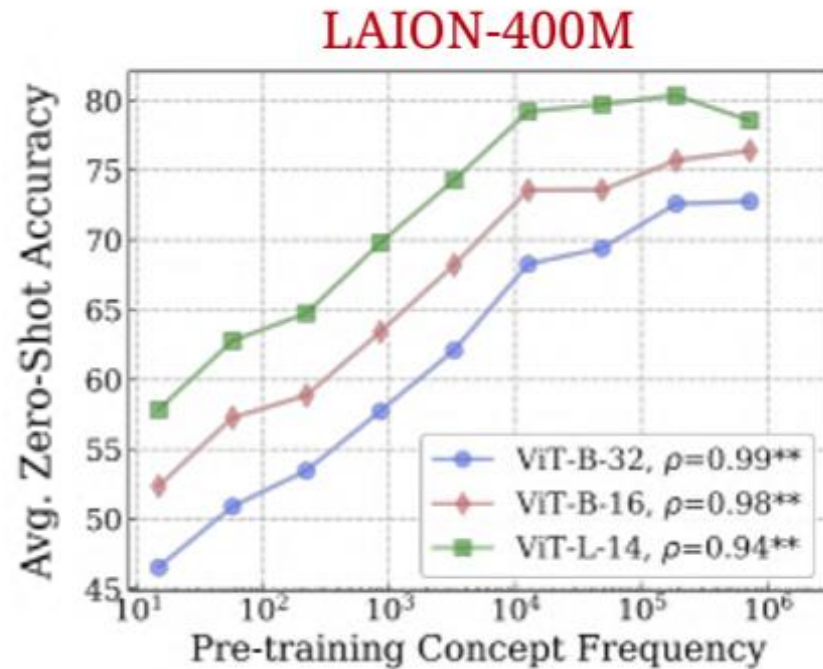
Classical, supervised  
scenario



Foundation models

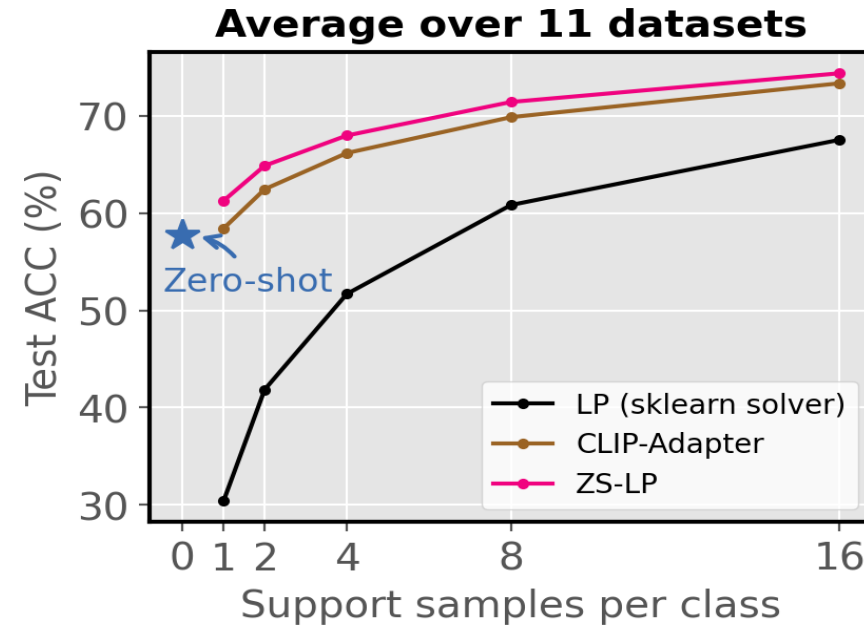
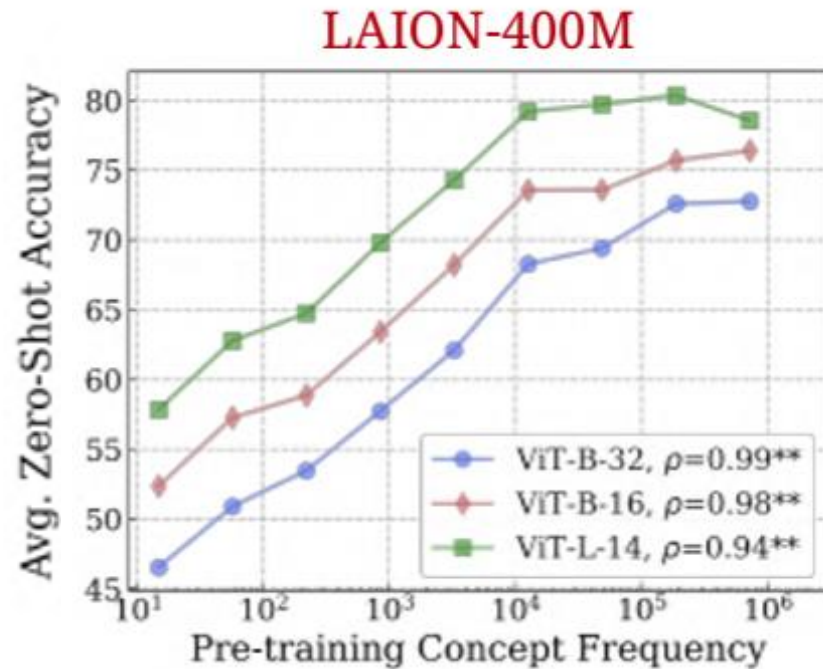
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# Conformal Prediction for Zero-Shot Models

- Transfer learning setting.



Tackled trough few-shot  
Linear Probing

Plot 1 from [Udandaro et al., No “Zero-Shot” Without Exponential Data: Pretraining Concept Frequency Determines Multimodal Model Performance, NeurIPS 2024]

Plot 2 from [Silva-Rodríguez et al., A Closer Look at the Few-Shot Adaptation of Large Vision-Language Models, CVPR 2024]

# Conformal Prediction for Zero-Shot Models

- Can we adapt and conformalize using the same data?



# Conformal Prediction for Zero-Shot Models

- Can we adapt and conformalize using the same data?



- Training a Linear Probe on the logit space

$$\mathcal{D}_{\text{cal}} = \{(\mathbf{l}_i, y_i)\}_{i=1}^N \quad \mathcal{D}_{\text{test}} = \{(\mathbf{l}_i, )\}_{i=N+1}^{N+M}$$

- New class prototypes on the logit projections are defined  $\mathbf{W} \in \mathbb{R}^{K \times K}$ .

- These obtain new class scores based on the **temperature-scaled Euclidean distance**  $l'_k = -\frac{\tau^{\text{LP}}}{2} \|\mathbf{l} - \mathbf{w}_k\|$ .

- Using calibration data, optimize the class prototypes to **minimize cross-entropy loss**.

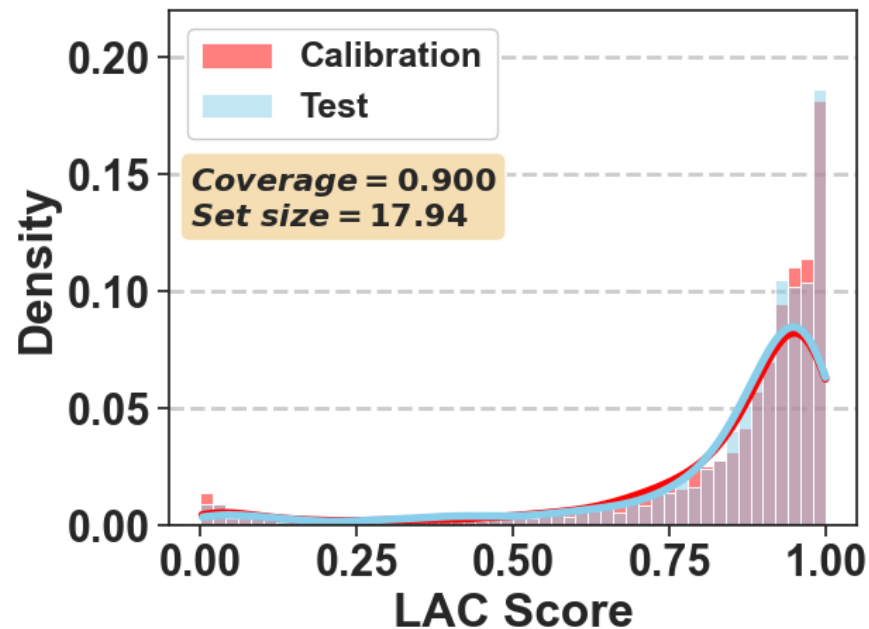
$$\min_{\mathbf{W}} -\frac{1}{NK} \sum_{i=1}^I \sum_{k=1}^K y_{ik} \log p_{ik},$$

# Conformal Prediction for Zero-Shot Models

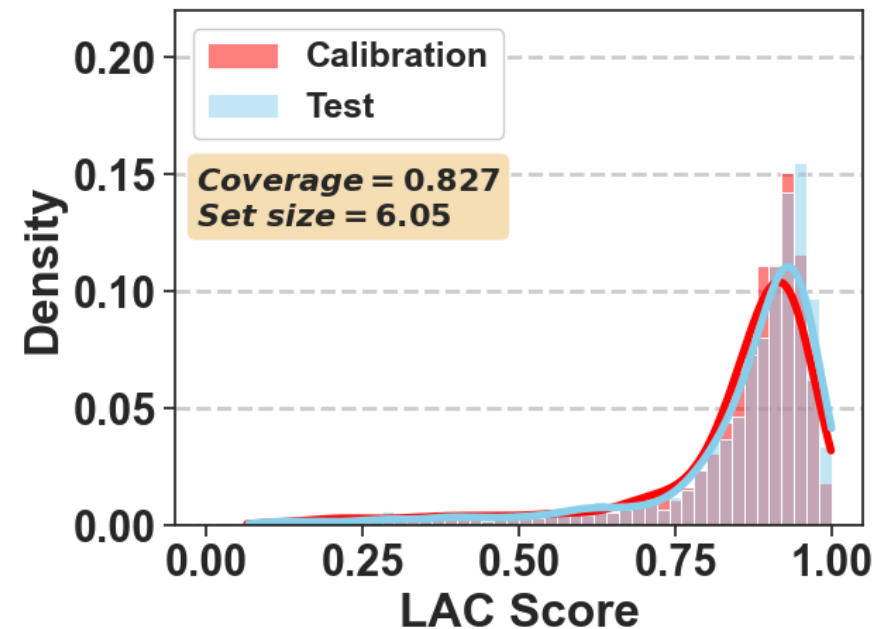
- Can we adapt and conformalize using the same data?



- Conformal Prediction performance



Zero-shot



Adapt + Conformalize in Calibration

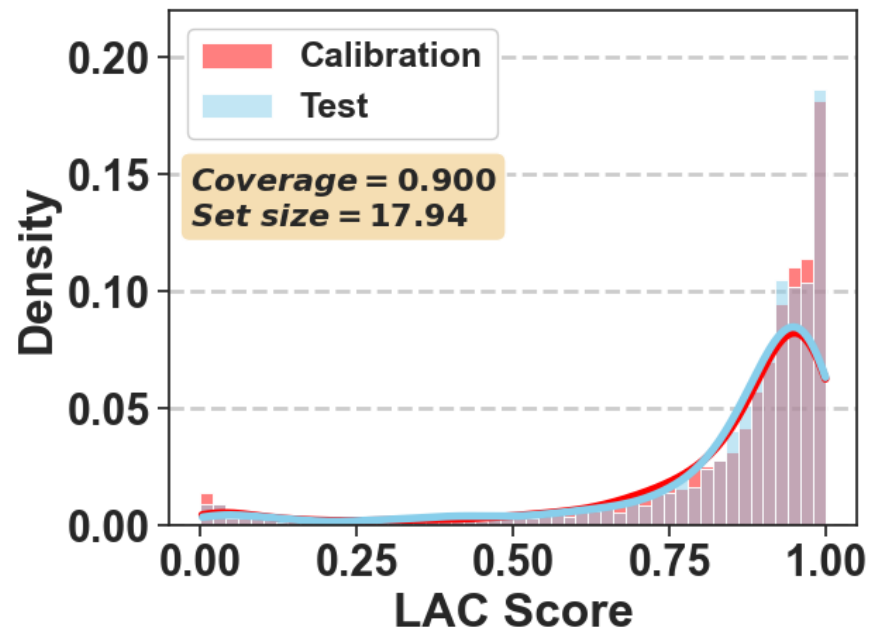


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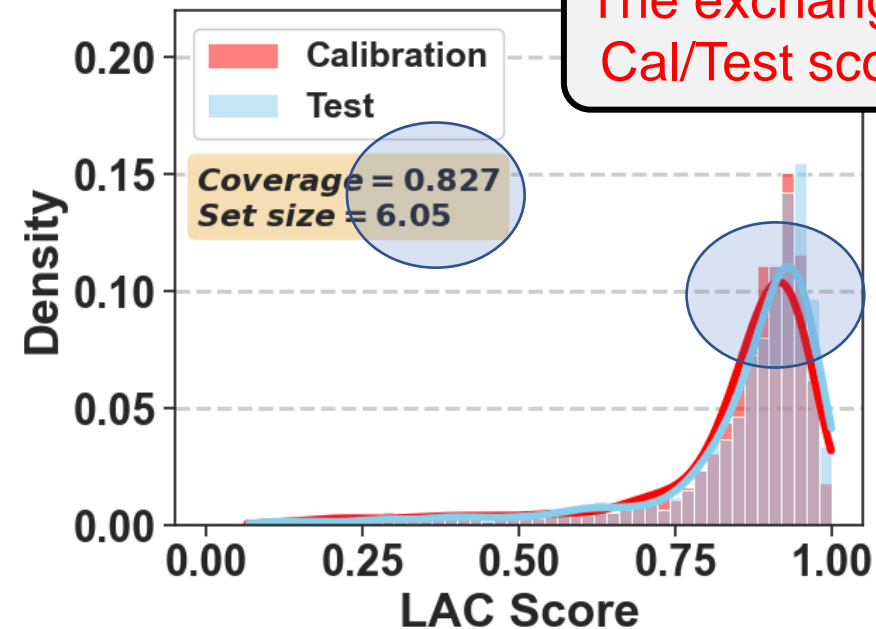
- Can we adapt and conformalize using the same data?



- Conformal Prediction performance



Zero-shot



Adapt + Conformalize in Calibration

The exchangeability of the Cal/Test scores is broken

# Conformal Prediction for Zero-Shot Models

## ▪ Transfer Learning for Conformal Prediction

1. Does not directly rely on Cal labels.

Unsupervised

$$\mathcal{D}_{\text{cal}} = \{(\mathbf{l}_i, y_i)\}_{i=1}^N$$



# Conformal Prediction for Zero-Shot Models

## ▪ Transfer Learning for Conformal Prediction

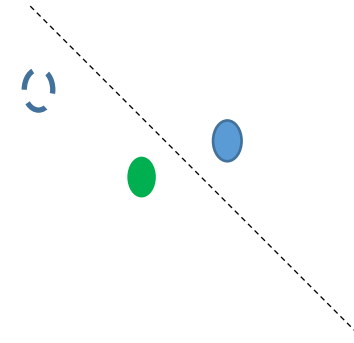
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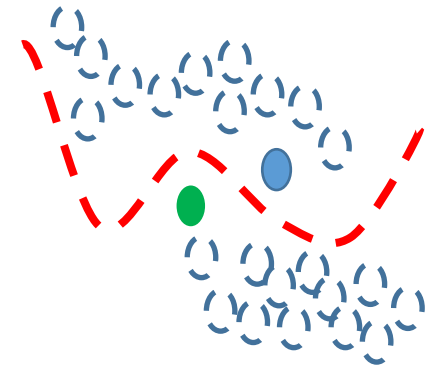
$$\mathcal{D}_{\text{cal}} = \{(\mathbf{l}_i, y_i)\}_{i=1}^N$$

2. Jointly modifies Cal/Test score distributions.

Transductive



**Inductive**  
One test sample  
at a time



**Transductive**  
Joint test-time  
prediction

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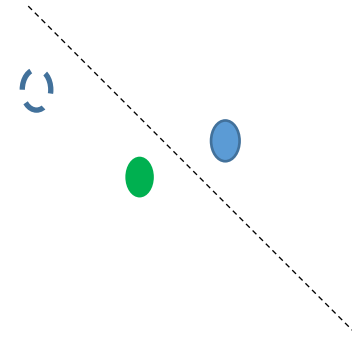
$$\mathcal{D}_{\text{cal}} = \{(\mathbf{l}_i, y_i)\}_{i=1}^N$$

2. Jointly modifies Cal/Test score distributions.

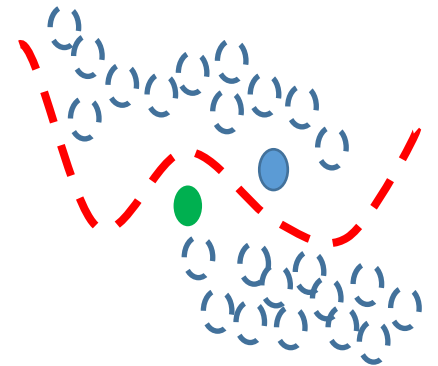
Transductive

▪ Similarity matrix.

$$\mathbf{S} \in \mathbb{R}^{K \times (N+M)} = [l_{ki}]_{k=1, i=1}^{k=K, i=N+M}$$



**Inductive**  
One test sample  
at a time



**Transductive**  
Joint test-time  
prediction

# Conformal Prediction for Zero-Shot Models

## ■ Conformal Optimal Transport

**Learning goal:** find the joint probability matrix (codes) which maximize the similarity assignment.

$$\max_{\mathbf{Q} \in \mathcal{Q}} \text{tr}(\mathbf{Q}^\top \mathbf{S})$$

where  $\mathbf{Q} \in \mathbb{R}_+^{K \times (N+M)}$  is the assignment matrix, formed by individual codes for each sample,  $\mathbf{q}_i$ .

---

**Algorithm 1** Conf-OT conformal prediction.

---

```

1: input: calibration dataset  $\mathcal{D}_{\text{cal}} = \{(l_i, y_i)\}_{i=1}^N$ , query
   set  $\mathcal{D}_{\text{test}} = \{(l_i)\}_{i=N+1}^{N+M}$ , non-conformity score function
    $\mathcal{S}$ , error level  $\alpha$ , entropic weight  $\tau$ , iterations  $T$ .
   // Block 1. - Transductive transfer learning.
   // Step 1.1. - Init. optimal transport problem.
2:  $\mathbf{S} \in \mathbb{R}^{K \times (N+M)} = [l_{ki}]_{k=1, i=1}^{k=K, i=N+M}$  // Sim. matrix.
3:  $\mathbf{m} = \frac{1}{N} \sum_1^N y_i^{\text{obs}}$  // Label-marginal.
4:  $\mathbf{u}_{(N+M)} = \frac{1}{(N+M)} \mathbf{1}_{(N+M)}$  // Sample marginal.
   // Step 1.2. - Compute renormalization vectors.
5:  $\mathbf{Q}^{(0)} = (\exp(\mathbf{S}/\tau) / \sum(\exp(\mathbf{S}/\tau)))$  // Init. codes.
6:  $\mathbf{c}^{(0)} = \mathbf{1}_{(N+M)}$  // Init. renormalization vector.
7: for  $t$  in  $[1, \dots, T]$  do
8:    $\mathbf{r}^{(t)} = \mathbf{m} / (\mathbf{Q}^{(0)} \mathbf{c}^{(t-1)})$  // Eq. (9).
9:    $\mathbf{c}^{(t)} = \mathbf{u}_{(N+M)} / (\mathbf{Q}^{(0)} \mathbf{r}^{(t)})$  // Eq. (10).
10: end for
   // Step 1.3. - Compute codes.
11:  $\mathbf{Q}^* = \text{Diag}(\mathbf{r}^{(T)}) \mathbf{Q}^{(0)} \text{Diag}(\mathbf{c}^{(T)})$  // Transport codes.
12:  $\mathbf{Q}^* = \mathbf{Q}^* \text{Diag}(1 / \sum_k q_{ki}^*)$  // Normalize.
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13:  $\mathcal{D}_{\text{cal}} = \{(q_i^{*\top}, y_i)\}_{i=1}^N$ ,  $\mathcal{D}_{\text{test}} = \{(q_i^{*\top})\}_{i=N+1}^{N+M}$ 
   // Step 2.1. -  $1 - \alpha$  non-conformity score quantile.
14:  $\{s_i\}_{i=1}^N = \{\mathcal{S}(q_i^{*\top}, y_i)\}_{i=1}^N$  // Non-conformity scores.
15:  $\hat{s} \leftarrow \{s_i\}_{i=1}^N, \alpha$  // Search threshold - Eq. (3).
   // Step 2.2. - Create query sets.
16: return:  $\{\mathcal{C}(q_i^{*\top})\}_{i=N+1}^M$  // Eq. (4).

```

---

# Conformal Prediction for Zero-Shot Models

## ■ Conformal Optimal Transport

**Learning goal:** find the joint probability matrix (codes) which maximize the similarity assignment.

$$\max_{\mathbf{Q} \in \mathcal{Q}} \text{tr}(\mathbf{Q}^\top \mathbf{S})$$

where  $\mathbf{Q} \in \mathbb{R}_+^{K \times (N+M)}$  is the assignment matrix, formed by individual codes for each sample,  $\mathbf{Q}_i$ .

More concretely,  $\mathbf{Q}$  is restricted to be an element of the transportation polytope:

$$\mathcal{Q} = \{\mathbf{Q} \mid \mathbf{Q}\mathbf{1}_{(N+M)} = \mathbf{m}, \mathbf{Q}^\top \mathbf{1}_K = \mathbf{u}_{(N+M)}\}$$

---

**Algorithm 1** Conf-OT conformal prediction.

---

```

1: input: calibration dataset  $\mathcal{D}_{\text{cal}} = \{(l_i, y_i)\}_{i=1}^N$ , query
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marginals!

---

### Algorithm 1 Conf-OT conformal prediction.

---

```

1: input: calibration dataset  $\mathcal{D}_{\text{cal}} = \{(l_i, y_i)\}_{i=1}^N$ , query
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```

---

# Conformal Prediction for Zero-Shot Models

## ■ Conformal Optimal Transport

**Optimization:** We solve the linear program through the efficient Sinkhorn algorithm, which incorporates an **entropic-constraint**.

$$\max_{\mathbf{Q} \in \mathcal{Q}} \text{tr}(\mathbf{Q}^\top \mathbf{S}) + \varepsilon \mathcal{H}(\mathbf{Q})$$

---

**Algorithm 1** Conf-OT conformal prediction.

---

```

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---



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**Optimization:** We solve the linear program through the efficient Sinkhorn algorithm, which incorporates an **entropic-constraint**.

$$\max_{\mathbf{Q} \in \mathcal{Q}} \text{tr}(\mathbf{Q}^\top \mathbf{S}) + \varepsilon \mathcal{H}(\mathbf{Q})$$

Now, the soft codes  $\mathbf{Q}^*$  are the solution of the optimization problem, which can be efficiently optimized by computing marginal-renormalization vectors, such that:

$$\mathbf{Q}^* = \text{Diag}(\mathbf{r}^{(t)}) \mathbf{Q}^{(0)} \text{Diag}(\mathbf{c}^{(t)})$$

---

**Algorithm 1** Conf-OT conformal prediction.

---

```

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Norm S as  
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---

### Algorithm 1 Conf-OT conformal prediction.

---

```

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Incorporate  
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marginal

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Divide rows  
by initial label  
marginal

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13:  $\mathcal{D}_{\text{cal}} = \{(q_i^{* \top}, y_i)\}_{i=1}^N$ ,  $\mathcal{D}_{\text{test}} = \{(q_i^{* \top})\}_{i=N+1}^{N+M}$ 
   // Step 2.1. -  $1 - \alpha$  non-conformity score quantile.
14:  $\{s_i\}_{i=1}^N = \{\mathcal{S}(q_i^{* \top}, y_i)\}_{i=1}^N$  // Non-conformity scores.
15:  $\hat{s} \leftarrow \{s_i\}_{i=1}^N, \alpha$  // Search threshold - Eq. (3).
   // Step 2.2. - Create query sets.
16: return:  $\{\mathcal{C}(q_i^{* \top})\}_{i=N+1}^M$  // Eq. (4).
  
```

Divide columns by  
observed sample  
marginal

# Conformal Prediction for Zero-Shot Models

## ■ Conformal Optimal Transport

**Optimization:** We solve the linear program through the efficient Sinkhorn algorithm, which incorporates an **entropic-constraint**.

$$\max_{\mathbf{Q} \in \mathcal{Q}} \text{tr}(\mathbf{Q}^\top \mathbf{S}) + \varepsilon \mathcal{H}(\mathbf{Q})$$

Now, the soft codes  $\mathbf{Q}^*$  are the solution of the optimization problem, which can be efficiently optimized by computing marginal-renormalization vectors, such that:

$$\mathbf{Q}^* = \text{Diag}(\mathbf{r}^{(t)}) \mathbf{Q}^{(0)} \text{Diag}(\mathbf{c}^{(t)})$$

---

### Algorithm 1 Conf-OT conformal prediction.

---

```

1: input: calibration dataset  $\mathcal{D}_{\text{cal}} = \{(l_i, y_i)\}_{i=1}^N$ , query
   set  $\mathcal{D}_{\text{test}} = \{(l_i)\}_{i=N+1}^{N+M}$ , non-conformity score function
    $\mathcal{S}$ , error level  $\alpha$ , entropic weight  $\tau$ , iterations  $T$ .
   // Block 1. - Transductive transfer learning.
   // Step 1.1. - Init. optimal transport problem.
2:  $\mathbf{S} \in \mathbb{R}^{K \times (N+M)} = [l_{ki}]_{k=1, i=1}^{k=K, i=N+M}$  // Sim. matrix.
3:  $\mathbf{m} = \frac{1}{N} \sum_1^N \mathbf{y}_i^{\text{obs}}$  // Label-marginal.
4:  $\mathbf{u}_{(N+M)} = \frac{1}{(N+M)} \mathbf{1}_{(N+M)}$  // Sample marginal.
   // Step 1.2. - Compute renormalization vectors.
5:  $\mathbf{Q}^{(0)} = (\exp(\mathbf{S}/\tau) / \sum(\exp(\mathbf{S}/\tau)))$  // Init. codes.
6:  $\mathbf{c}^{(0)} = \mathbf{1}_{(N+M)}$  // Init. renormalization vector.
7: for  $t$  in  $[1, \dots, T]$  do
8:    $\mathbf{r}^{(t)} = \mathbf{m} / (\mathbf{Q}^{(0)} \mathbf{c}^{(t-1)})$  // Eq. (9).
9:    $\mathbf{c}^{(t)} = \mathbf{u}_{(N+M)} / (\mathbf{Q}^{(0)} \mathbf{r}^{(t)})$  // Eq. (10).
10: end for
   // Step 1.3. - Compute codes.
11:  $\mathbf{Q}^* = \text{Diag}(\mathbf{r}^{(T)}) \mathbf{Q}^{(0)} \text{Diag}(\mathbf{c}^{(T)})$  // Transport codes.
12:  $\mathbf{Q}^* = \mathbf{Q}^* \text{Diag}(1 / \sum_k q_{ki}^*)$  // Normalize.
   // Block 2. - Conformal prediction.
13:  $\mathcal{D}_{\text{cal}} = \{(l_i, y_i)\}_{i=1}^N$ 
   // Step 2.1. - Compute scores.
14:  $\{s_i\}_{i=1}^N = \{\mathcal{C}(q_i^*)\}_{i=1}^N$ 
15:  $\hat{s} \leftarrow \{s_i\}_{i=1}^N$ 
   // Step 2.2. - Create query sets.
16: return:  $\{\mathcal{C}(q_i^*)\}_{i=N+1}^{N+M}$  // Eq. (4).
```

---

Apply renorm. vectors  
and sample-wise.



# Conformal Prediction for Zero-Shot Models

## ■ Conformal Optimal Transport

**Conformal prediction**: we follow the standard SCP setting using codes instead of the original probabilities.

$$\mathcal{D}_{\text{cal}} = \{(\mathbf{q}_i, y_i)\}_{i=1}^N$$

$$\mathcal{D}_{\text{test}} = \{(\mathbf{q}_i, )\}_{i=N+1}^{N+M}$$

---

**Algorithm 1** Conf-OT conformal prediction.

---

```

1: input: calibration dataset  $\mathcal{D}_{\text{cal}} = \{(l_i, y_i)\}_{i=1}^N$ , query
   set  $\mathcal{D}_{\text{test}} = \{(l_i)\}_{i=N+1}^{N+M}$ , non-conformity score function
    $\mathcal{S}$ , error level  $\alpha$ , entropic weight  $\tau$ , iterations  $T$ .
   // Block 1. - Transductive transfer learning.
   // Step 1.1. - Init. optimal transport problem.
2:  $\mathbf{S} \in \mathbb{R}^{K \times (N+M)} = [l_{ki}]_{k=1, i=1}^{k=K, i=N+M}$  // Sim. matrix.
3:  $\mathbf{m} = \frac{1}{N} \sum_1^N \mathbf{y}_i^{\text{obs}}$  // Label-marginal.
4:  $\mathbf{u}_{(N+M)} = \frac{1}{(N+M)} \mathbf{1}_{(N+M)}$  // Sample marginal.
   // Step 1.2. - Compute renormalization vectors.
5:  $\mathbf{Q}^{(0)} = (\exp(\mathbf{S}/\tau) / \sum(\exp(\mathbf{S}/\tau)))$  // Init. codes.
6:  $\mathbf{c}^{(0)} = \mathbf{1}_{(N+M)}$  // Init. renormalization vector.
7: for  $t$  in  $[1, \dots, T]$  do
8:    $\mathbf{r}^{(t)} = \mathbf{m} / (\mathbf{Q}^{(0)} \mathbf{c}^{(t-1)})$  // Eq. (9).
9:    $\mathbf{c}^{(t)} = \mathbf{u}_{(N+M)} / (\mathbf{Q}^{(0)} \mathbf{r}^{(t)})$  // Eq. (10).
10: end for
   // Step 1.3. - Compute codes.
11:  $\mathbf{Q}^* = \text{Diag}(\mathbf{r}^{(T)}) \mathbf{Q}^{(0)} \text{Diag}(\mathbf{c}^{(T)})$  // Transport codes.
12:  $\mathbf{Q}^* = \mathbf{Q}^* \text{Diag}(1 / \sum_k q_{ki}^*)$  // Normalize.
   // Block 2. - Conformal prediction.
13:  $\mathcal{D}_{\text{cal}} = \{(q_i^{*\top}, y_i)\}_{i=1}^N$ ,  $\mathcal{D}_{\text{test}} = \{(q_i^{*\top})\}_{i=N+1}^{N+M}$ 
   // Step 2.1. -  $1 - \alpha$  non-conformity score quantile.
14:  $\{s_i\}_{i=1}^N = \{\mathcal{S}(q_i^{*\top}, y_i)\}_{i=1}^N$  // Non-conformity scores.
15:  $\hat{s} \leftarrow \{s_i\}_{i=1}^N, \alpha$  // Search threshold - Eq. (3).
   // Step 2.2. - Create query sets.
16: return:  $\{\mathcal{C}(q_i^{*\top})\}_{i=N+1}^M$  // Eq. (4).

```

# Conformal Prediction for Zero-Shot Models

## ■ Enhancing popular non-conformity scores

Method	$\alpha = 0.10$				$\alpha = 0.05$		
	Top-1 $\uparrow$	Cov	Size $\downarrow$	CCV $\downarrow$	Cov.	Size $\downarrow$	CCV $\downarrow$
<b>CLIP ResNet-50</b>							
LAC [42]	54.7	0.900	10.77	9.82	0.950	19.22	5.91
w/ Conf-OT	<b>57.3</b> <sub>+2.6</sub>	0.900	<b>8.61</b> <sub>-2.2</sub>	<b>9.15</b> <sub>-0.7</sub>	0.951	<b>15.53</b> <sub>-3.7</sub>	<b>5.61</b> <sub>-0.3</sub>
APS [54]	54.7	0.900	16.35	8.36	0.950	26.50	5.34
w/ Conf-OT	<b>57.3</b> <sub>+2.6</sub>	0.900	<b>12.94</b> <sub>-3.4</sub>	<b>7.64</b> <sub>-0.7</sub>	0.950	<b>20.96</b> <sub>-5.5</sub>	<b>5.03</b> <sub>-0.3</sub>
RAPS [2]	54.7	0.900	13.37	8.46	0.950	22.06	5.44
w/ Conf-OT	<b>57.3</b> <sub>+2.6</sub>	0.900	<b>11.17</b> <sub>-2.2</sub>	<b>7.72</b> <sub>-0.7</sub>	0.950	<b>17.24</b> <sub>-4.8</sub>	<b>5.19</b> <sub>-0.3</sub>
<b>CLIP ViT-B/16</b>							
LAC [42]	63.8	0.899	5.52	10.37	0.950	10.24	6.14
w/ Conf-OT	<b>66.7</b> <sub>+2.9</sub>	0.900	<b>4.40</b> <sub>-1.1</sub>	<b>9.48</b> <sub>-0.9</sub>	0.949	<b>7.99</b> <sub>-2.3</sub>	<b>5.80</b> <sub>-0.3</sub>
APS [54]	63.8	0.900	9.87	8.39	0.950	16.92	5.51
w/ Conf-OT	<b>66.7</b> <sub>+2.9</sub>	0.899	<b>7.64</b> <sub>-2.2</sub>	<b>7.44</b> <sub>-1.0</sub>	0.949	<b>12.58</b> <sub>-4.3</sub>	<b>5.09</b> <sub>-0.4</sub>
RAPS [2]	63.8	0.900	8.12	8.50	0.950	12.66	5.52
w/ Conf-OT	<b>66.7</b> <sub>+2.9</sub>	0.900	<b>6.68</b> <sub>-1.4</sub>	<b>7.48</b> <sub>-1.0</sub>	0.949	<b>10.11</b> <sub>-2.6</sub>	<b>5.16</b> <sub>-0.4</sub>

# Conformal Prediction for Zero-Shot Models

- Enhancing popular non-conformity scores

Method	$\alpha = 0.10$				$\alpha = 0.05$		
	Top-1 $\uparrow$	Cov	Size $\downarrow$	CCV $\downarrow$	Cov	Size $\downarrow$	CCV $\downarrow$
<b>CLIP ResNet-50</b>							
LAC [42]	54.7	0.900	10.77	9.82	0.950	19.22	5.91
w/ Conf-OT	57.3 <sub>+2.6</sub>	0.900	8.61 <sub>-2.2</sub>	9.15 <sub>-0.7</sub>	0.951	15.53 <sub>-3.7</sub>	5.61 <sub>-0.3</sub>
APS [54]	54.7	0.900	16.35	8.36	0.950	26.50	5.34
w/ Conf-OT	57.3 <sub>+2.6</sub>	0.900	12.94 <sub>-3.4</sub>	7.64 <sub>-0.7</sub>	0.950	20.96 <sub>-5.5</sub>	5.03 <sub>-0.3</sub>
RAPS [2]	54.7	0.900	13.37	8.46	0.950	22.06	5.44
w/ Conf-OT	57.3 <sub>+2.6</sub>	0.900	11.17 <sub>-2.2</sub>	7.72 <sub>-0.7</sub>	0.950	17.24 <sub>-4.8</sub>	5.19 <sub>-0.3</sub>
<b>CLIP ViT-B/16</b>							
LAC [42]	63.8	0.899	5.52	10.37	0.950	10.24	6.14
w/ Conf-OT	66.7 <sub>+2.9</sub>	0.900	4.40 <sub>-1.1</sub>	9.48 <sub>-0.9</sub>	0.949	7.99 <sub>-2.3</sub>	5.80 <sub>-0.3</sub>
APS [54]	63.8	0.900	9.87	8.39	0.950	16.92	5.51
w/ Conf-OT	66.7 <sub>+2.9</sub>	0.899	7.64 <sub>-2.2</sub>	7.44 <sub>-1.0</sub>	0.949	12.58 <sub>-4.3</sub>	5.09 <sub>-0.4</sub>
RAPS [2]	63.8	0.900	8.12	8.50	0.950	12.66	5.52
w/ Conf-OT	66.7 <sub>+2.9</sub>	0.900	6.68 <sub>-1.4</sub>	7.48 <sub>-1.0</sub>	0.949	10.11 <sub>-2.6</sub>	5.16 <sub>-0.4</sub>

Valid coverage!

15-20% better



# Conformal Prediction for Zero-Shot Models

## ■ Comparison to popular transductive methods

Method	$\alpha = 0.10$					
	Top-1 $\uparrow$	T	GPU	Cov.	Size $\downarrow$	CCV $\downarrow$
LAC [42]	63.8	<b>0.42</b>	-	0.899	5.52	10.37
$\text{TIM}_{\text{KL}(\widehat{\mathbf{m}}  \mathbf{u}_K)}$ [6]	$64.7_{+0.9}$	11.05	8.24	0.899	$8.30_{+2.8}$	$10.41_{+0.0}$
$\text{TIM}_{\text{KL}(\widehat{\mathbf{m}}  \mathbf{m})}$ [6]	$65.0_{+1.2}$	11.03	8.24	0.898	$7.73_{+2.2}$	$10.89_{+0.5}$
TransCLIP [74]	$65.1_{+1.3}$	12.00	12.2	<b>0.892</b>	$5.76_{+0.2}$	$11.02_{+0.7}$
Conf-OT	<b><math>66.7_{+2.9}</math></b>	0.61	-	0.900	<b><math>4.40_{-1.1}</math></b>	<b><math>9.48_{-0.9}</math></b>

TIM from [Boudiaf et al., Transductive Information Maximization for Few-Shot Learning, NeurIPS 2020]

TransCLIP from [Zanella et al., Boosting Vision-Language Models with Transduction, NeurIPS 2024]

# Conformal Prediction for Zero-Shot Models

## ■ Comparison to popular transductive methods

Method	$\alpha = 0.10$					
	Top-1 $\uparrow$	T	GPU	Cov.	Size $\downarrow$	CCV $\downarrow$
LAC [42]	63.8	<b>0.42</b>	-	0.899	5.52	10.37
$\text{TIM}_{\text{KL}(\widehat{\mathbf{m}}  \mathbf{u}_K)}$ [6]	64.7 <sub>+0.9</sub>	11.05	8.24	0.899	8.30 <sub>+2.8</sub>	10.41 <sub>+0.0</sub>
$\text{TIM}_{\text{KL}(\widehat{\mathbf{m}}  \mathbf{m})}$ [6]	65.0 <sub>+1.2</sub>	11.03	8.24	0.898	7.73 <sub>+2.2</sub>	10.89 <sub>+0.5</sub>
TransCLIP [74]	65.1 <sub>+1.3</sub>	12.00	12.2	<b>0.892</b>	5.76 <sub>+0.2</sub>	11.02 <sub>+0.7</sub>
Conf-OT	<b>66.7<sub>+2.9</sub></b>	0.61	-	0.900	<b>4.40<sub>-1.1</sub></b>	<b>9.48<sub>-0.9</sub></b>

no improvement

training-free

Better than SoTA even in the  
discriminative aspect!

TIM from [Boudiaf et al., Transductive Information Maximization for Few-Shot Learning, NeurIPS 2020]

TransCLIP from [Zanella et al., Boosting Vision-Language Models with Transduction, NeurIPS 2024]

# Conformal Prediction for Zero-Shot Models

## ■ Evaluation of the data-efficiency

Method	Ratio	Top-1↑	$\alpha = 0.10$		
			Cov.	Size↓	CCV↓
LAC	0.1 - 0.9	63.8	0.903	7.71	9.65
	0.2 - 0.8	63.8	0.899	5.56	9.80
	0.5 - 0.5	63.8	0.899	5.52	10.37
	0.8 - 0.2	63.8	0.899	5.56	11.70
Conf-OT+LAC	0.1 - 0.9	66.6	0.901	4.53	8.73
	0.2 - 0.8	66.7	0.899	4.39	8.86
	0.5 - 0.5	66.7	0.900	4.40	9.48
	0.8 - 0.2	66.7	0.899	4.41	11.12

**Robustness to small  
calibration sets**

Method	M	Top-1↑	$\alpha = 0.10$		
			Cov.	Size↓	CCV↓
LAC	-	63.8	0.899	5.52	10.37
w/ Conf-OT	Full	66.7	0.900	4.40	9.48
w/ Conf-OT	32	66.5	0.898	4.43	9.66
w/ Conf-OT	16	66.5	0.898	4.43	9.67
w/ Conf-OT	8	66.6	0.898	4.42	9.67

**Robustness to small  
query inputs**

# Conformal Prediction for Zero-Shot Models

## ■ Evaluation of the data-efficiency

Method	Ratio	Top-1↑	$\alpha = 0.10$		
			Cov.	Size↓	CCV↓
LAC	0.1 - 0.9	63.8	0.903	7.71	9.65
	0.2 - 0.8	63.8	0.899	5.56	9.80
	0.5 - 0.5	63.8	0.899	5.52	10.37
	0.8 - 0.2	63.8	0.899	5.56	11.70
Conf-OT+LAC	0.1 - 0.9	66.6	0.901	4.53	8.73
	0.2 - 0.8	66.7	0.899	4.39	8.86
	0.5 - 0.5	66.7	0.900	4.40	9.48
	0.8 - 0.2	66.7	0.899	4.41	11.12

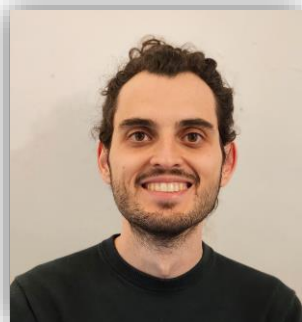
**Robustness to small  
calibration sets**

Method	M	Top-1↑	$\alpha = 0.10$		
			Cov.	Size↓	CCV↓
LAC	-	63.8	0.899	5.52	10.37
w/ Conf-OT	Full	66.7	0.900	4.40	9.48
w/ Conf-OT	32	66.5	0.898	4.43	9.66
w/ Conf-OT	16	66.5	0.898	4.43	9.67
w/ Conf-OT	8	66.6	0.898	4.42	9.67

**Robustness to small  
query inputs**

# Conformal Prediction for Zero-Shot Models

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