



UQinMIA – Sept 2025

# **Uncertainty Quantification for Medical Foundation Models**



Julio Silva-Rodríguez



Ismail Ben Ayed



Jose Dolz

# Outline

## A. Vision-Language Models (VLMs)

- Contrastive Language-Image Pre-training (CLIP).
- Zero-shot and few-shot inference.
- Calibration in contrastive VLMs.
- Vision-language models for medical imaging.

#### **B.** Conformal Prediction in VLMs

- Split conformal prediction (SCP).
- Theoretical guarantees in CP.
- Benefits of foundation models for CP.
- Full conformal predictors.
- Full conformal adaptation (FCA).
- Interpretability of conformal sets.

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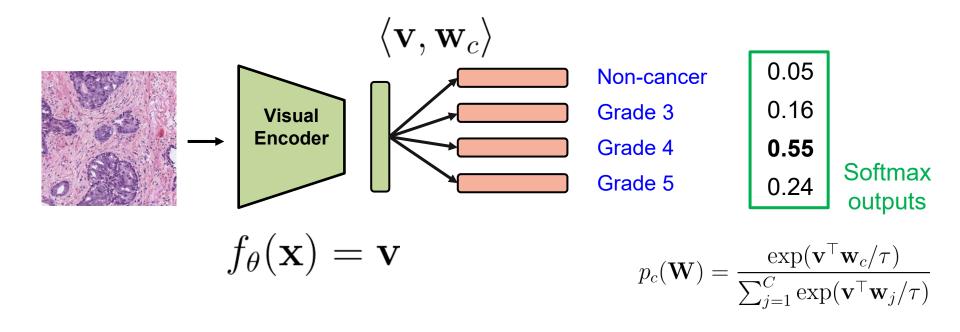
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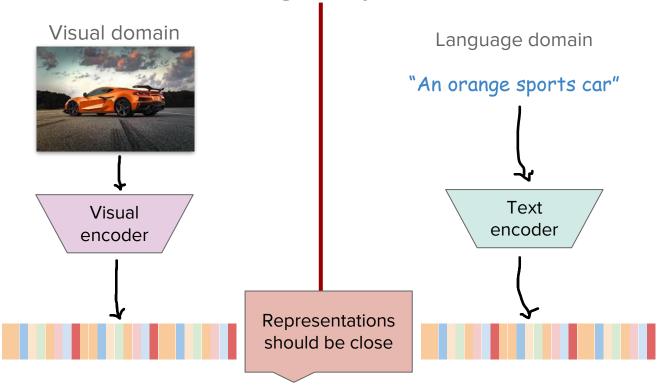
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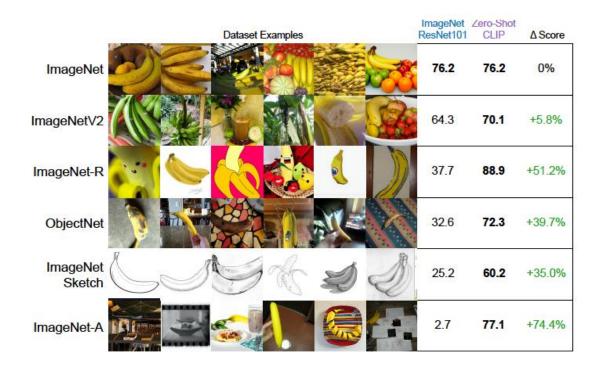
## **Dataset-focused image classifiers**



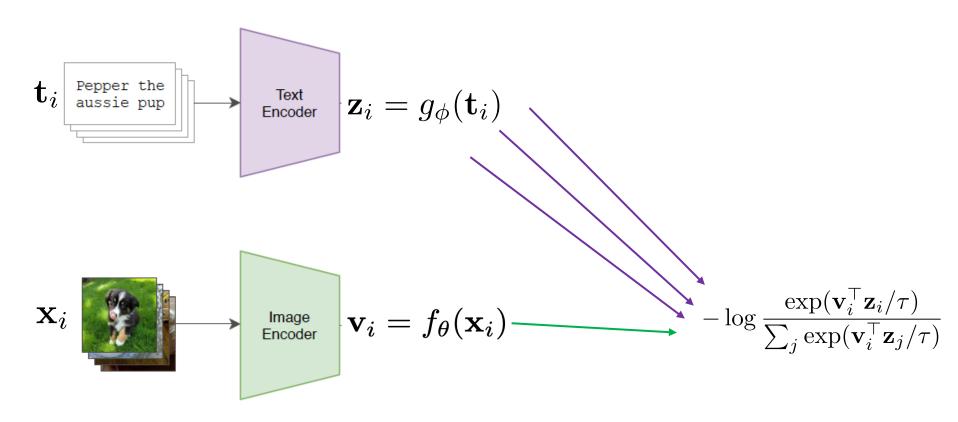
# Foundational Vision-Language Models (VLMs) are transforming computer vision



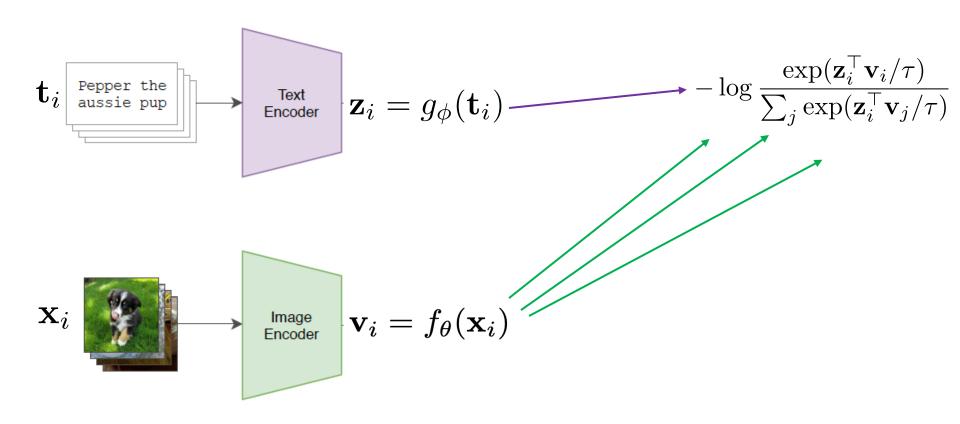
# Promising zero-shot generalization (in comparison to standard task-specific learning)



## **Contrastive Language-Image Pre-training (CLIP)**

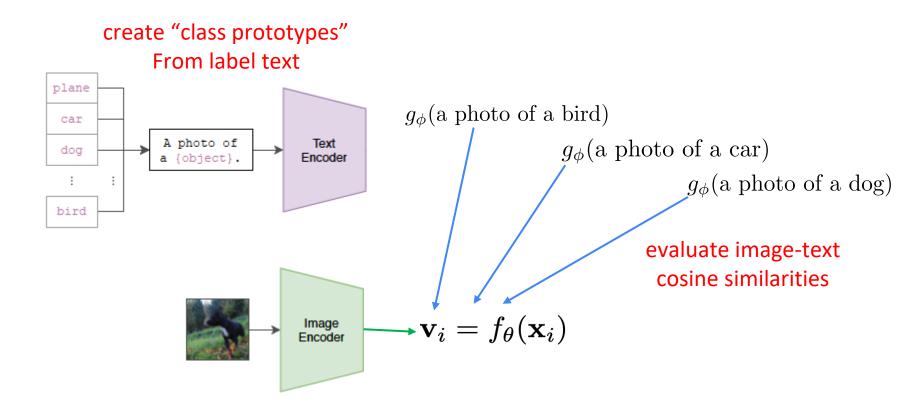


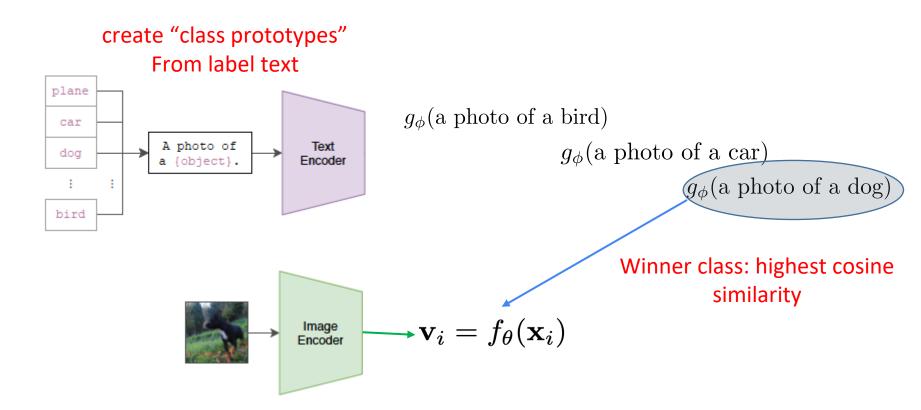
# **Contrastive Language-Image Pre-training (CLIP)**

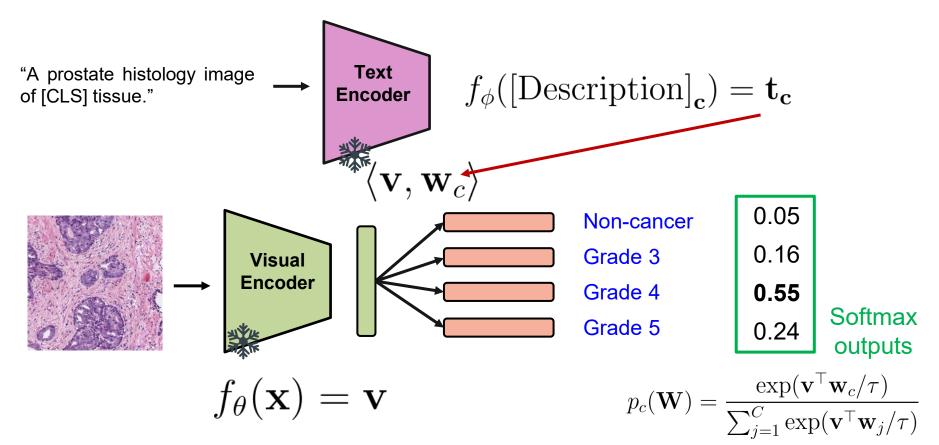


# create "class prototypes" From label text

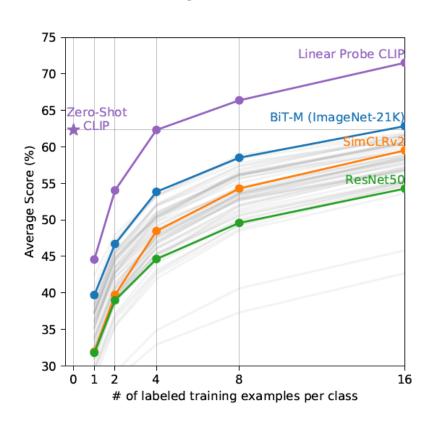


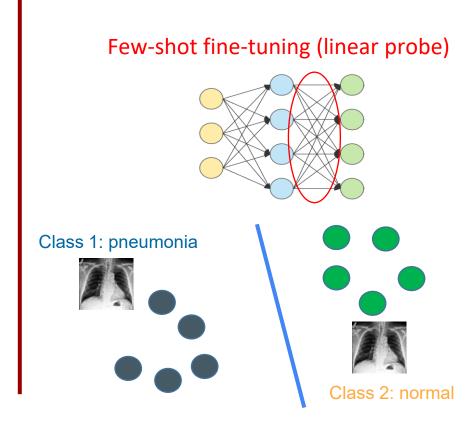




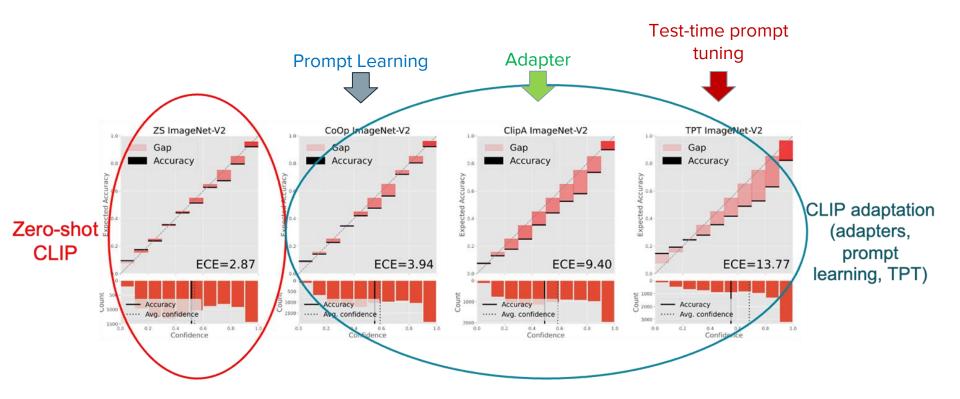


## **Beyond zero-shot: Few-shot generalization**





## **Calibration in contrastive VLMs**



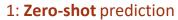
## **Calibration in contrastive VLMs**

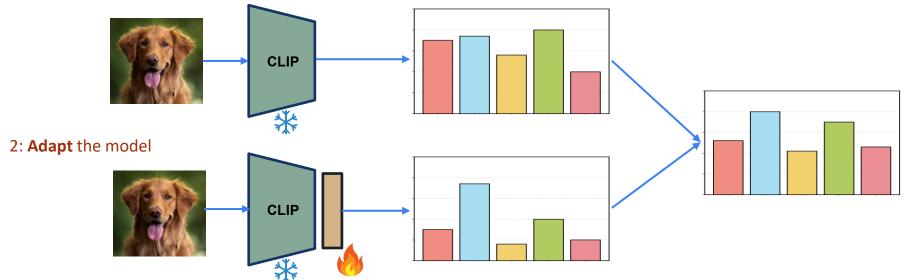
minimize 
$$\mathcal{H}(\boldsymbol{Y}, \boldsymbol{P})$$

subject to 
$$l_i^{\text{ZS-min}} \mathbf{1} \leq$$

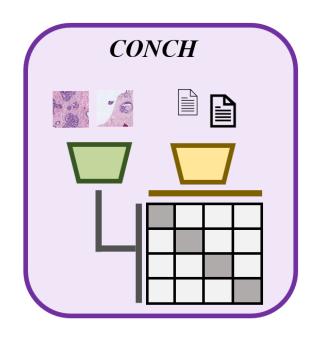
$$l_i^{ ext{ZS-min}} \mathbf{1} \leq oldsymbol{l}_i \leq l_i^{ ext{ZS-max}} \mathbf{1}$$

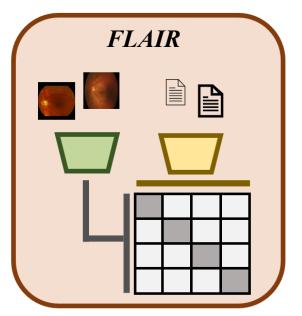


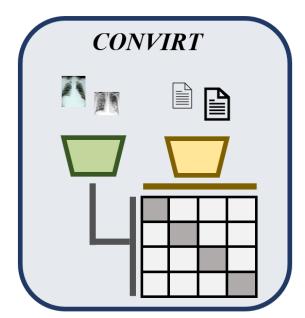




# **Medical Vision-Language Models**

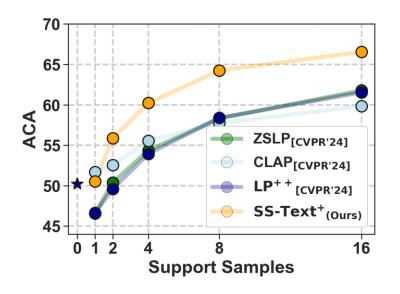


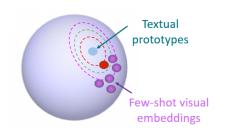


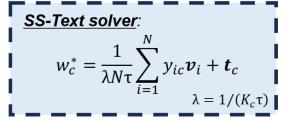


## **Medical Vision-Language Models**

$$\min_{\mathbf{W}} \mathcal{L}(\mathbf{W}) = -\frac{1}{N} \sum_{i=1}^{N} \sum_{c=1}^{C} y_{ic} \ln(p_{ic}(\mathbf{W})) + \frac{\lambda}{2} \sum_{c=1}^{C} ||\mathbf{w}_{c} - \mathbf{t}_{c}||_{2}^{2}.$$







# Outline

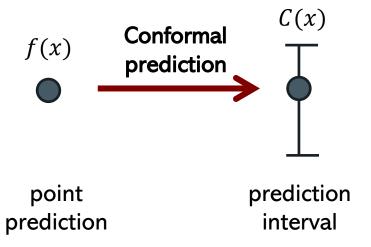
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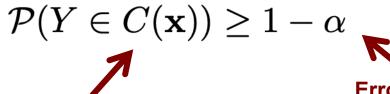
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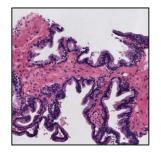
# **Conformal Prediction (CP)**



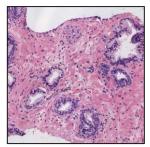
# **Conformal Prediction (CP)**







GT: NC Set: [NC]

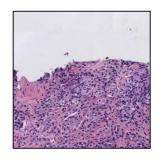


Sets

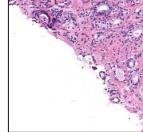
**GT**: G3 **Set**: [G3]



**GT**: G3 **Set**: [G3,G4]



**GT**: G5 **Set**: [G5]

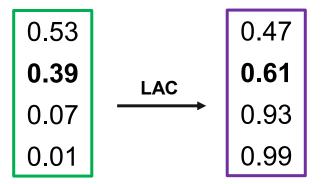


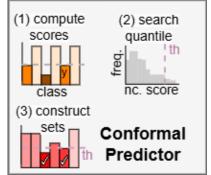
**GT**: G5

**Set**: [G3,G4,G5]

1. Non-conformity score from black-box classifier.

$$\mathcal{S}(\mathbf{x}, y) = 1 - \hat{p}_{k=y}$$



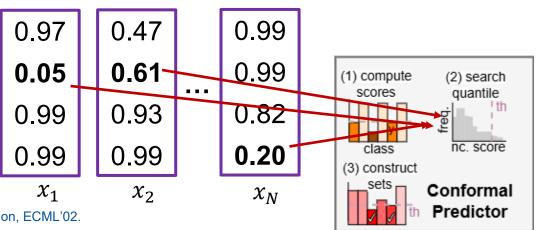


 $S(\mathbf{x}, y) = 1 - \hat{p}_{k=y}$ 1. Non-conformity score from black-box classifier.

$$\mathcal{S}(\mathbf{x}, y) = 1 - \hat{p}_{k=y}$$

2. Search threshold in the **true-label** S(x, y) distribution that ensures a given coverage.



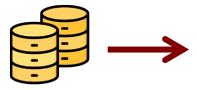


Papadopoulos et al. Inductive confidence machines for regression, ECML'02. Vovk et al. Algorithmic learning in a random world, Springer'05.

1. Non-conformity score from black-box classifier.  $~\mathcal{S}(\mathbf{x},y) =$ 

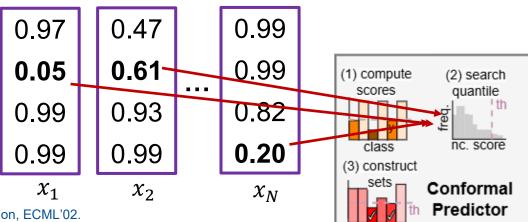
$$\mathcal{S}(\mathbf{x}, y) = 1 - \hat{p}_{k=y}$$

2. Search threshold in the **true-label** S(x, y) distribution that ensures a given coverage.



$$\hat{s} = \inf \left[ s : \frac{|i \in \{1, ..., N\} : s_i \le s|}{N} \ge \frac{\lceil (N+1)(1-\alpha) \rceil}{N} \right]$$

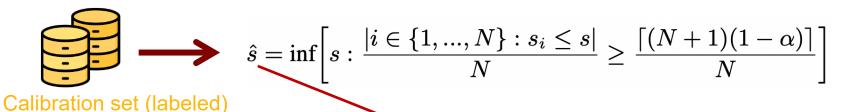
Calibration set (labeled)



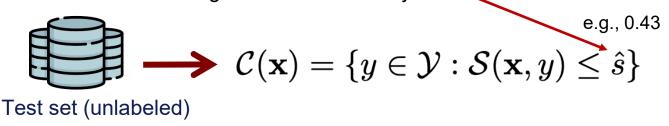
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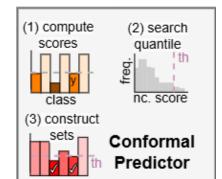
1. Non-conformity score from black-box classifier.  $~\mathcal{S}(\mathbf{x},y)=1-\hat{p}_{k=y}$ 

2. Search threshold in the **true-label** S(x, y) distribution that ensures a given coverage.



3. Create sets using the threshold as rejection criteria.



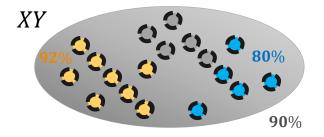


$$\mathcal{P}(Y \in C(\mathbf{x})) \ge 1 - \alpha$$

- 1. Distribution-free, e.g., no gaussian distribution required.
- **2. Marginal over** *XY*, i.e., does not inform about specific examples/subgroups.
- **3.** Assumes at least **exchangeability** of  $D_{cal}$  and  $D_{test}$ .
- **4. Finite-sample guarantee** holds on average across random experiments.

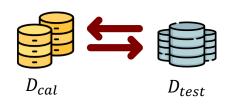
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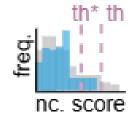
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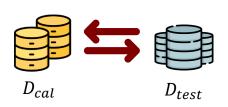
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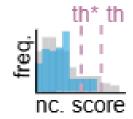


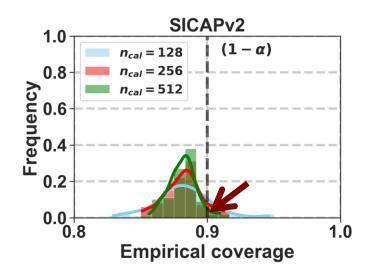


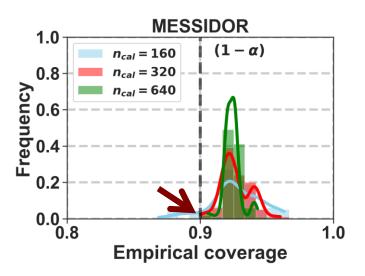
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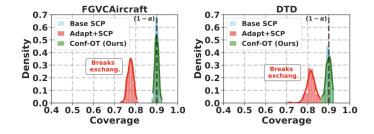




Are data samples coming from different patients necessary exchangeable?

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

- 1. Distribution-free, e.g., no gaussian distribution required.
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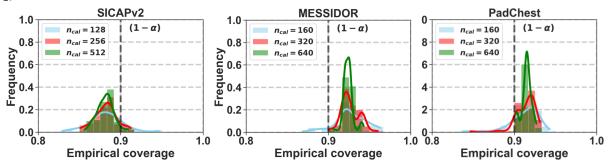
$$\mathcal{P}(Y \in C(\mathbf{x})) \ge 1 - \alpha$$

Marques F. Universal distribution of the empirical coverage in split conformal prediction, ArXiv'24.

**Theorem 1.** Under the data exchangeability assumption, for a regular conformity function, the sequence of coverage indicators  $\{Z_i\}_{i\geq 1}$  is exchangeable and  $m\times C_m^{(n,\alpha)}$  is distributed as a Beta-Binomial( $\lceil (1-\alpha)(n+1)\rceil$ ,  $\lfloor \alpha(n+1)\rfloor$ ) random variable, to the effect that the distribution of the empirical coverage is given by

$$P\left(C_m^{(n,\alpha)} = \frac{k}{m}\right) = \binom{m}{k} \frac{n! \left(k + \lceil (1-\alpha)(n+1)\rceil - 1\right)! \left(m - k + \lfloor \alpha(n+1)\rfloor - 1\right)!}{\left(\lceil (1-\alpha)(n+1)\rceil - 1\right)! \left(\lfloor \alpha(n+1)\rfloor - 1\right)! \left(m + n\right)!},$$

**Theorem 2.** Under the data exchangeability assumption, for a regular conformity function, the empirical coverage  $C_m^{(n,\alpha)}$  converges almost surely, when the future batch size tends to infinity, to a random variable  $C_{\infty}^{(n,\alpha)}$  with distribution  $Beta(\lceil (1-\alpha)(n+1)\rceil, \lfloor \alpha(n+1)\rfloor)$ .



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

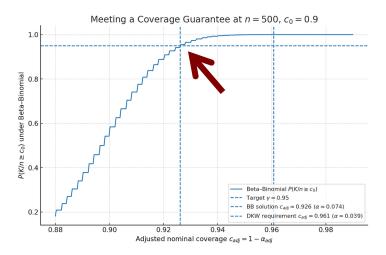
"I guarantee you predictive sets with coverage of 90%, with a probability of at least 95%, and a 1% tolerance error"

		7						1				
	$\epsilon = 0.1$			$\epsilon = 0.05$			$\epsilon = 0.01$			$\epsilon = 0.005$		
$\tau$ $1-\alpha$	90%	95%	99%	90%	95%	99%	90%	95%	99%	90%	95%	99%
80%	40	57	98	170	241	418	4,326	6,142	10,611	17,314	24,581	42,457
85%	30	42	77	134	189	330	3,446	4,893	8,451	13,794	19,587	33,830
90%	11	14	47	90	128	227	2,429	3,448	5,958	9,733	13,821	23,875
95%	19	19	29	22	29	97	1,270	1,806	3,132	5,125	7,278	12,578

Marques F. Universal distribution of the empirical coverage in split conformal prediction, ArXiv'24.

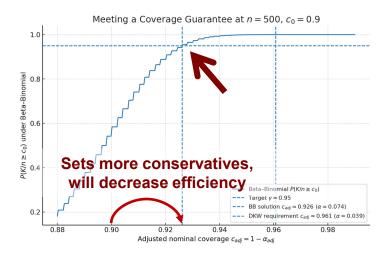
$$\mathcal{P}(Y \in C(\mathbf{x})) \ge 1 - \alpha$$

"I want predictive sets with coverage above 90%, with a probability of at least 95%, and a 1% tolerance error. I have N=500 calibration samples: which nominal coverage should I use?"



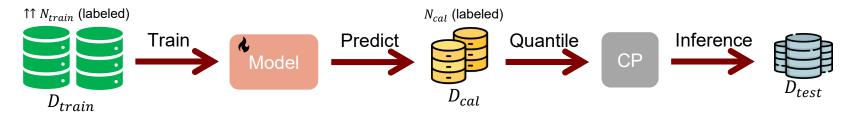
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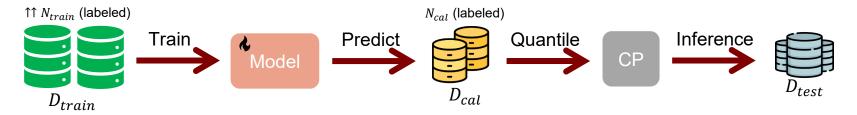


# Foundation models and conformal prediction

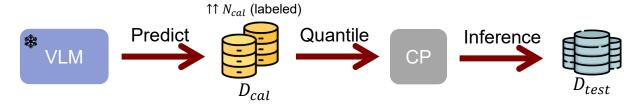
1. Standard task-specific training scenario.



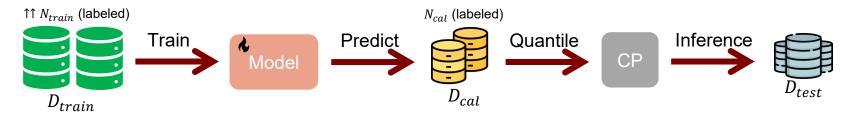
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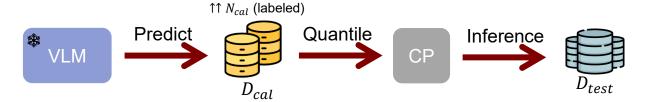
Modern scenario with zero-shot VLMs.



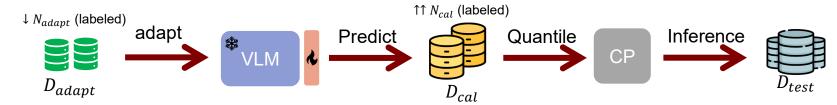
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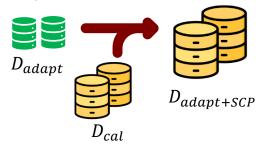


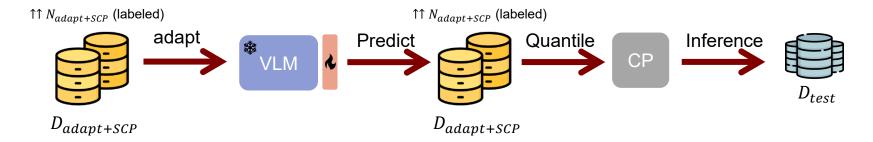
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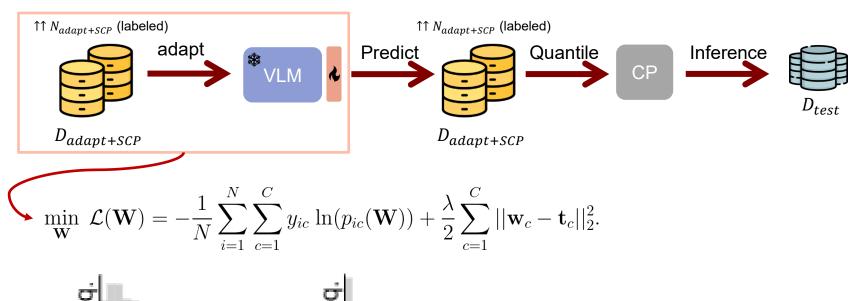


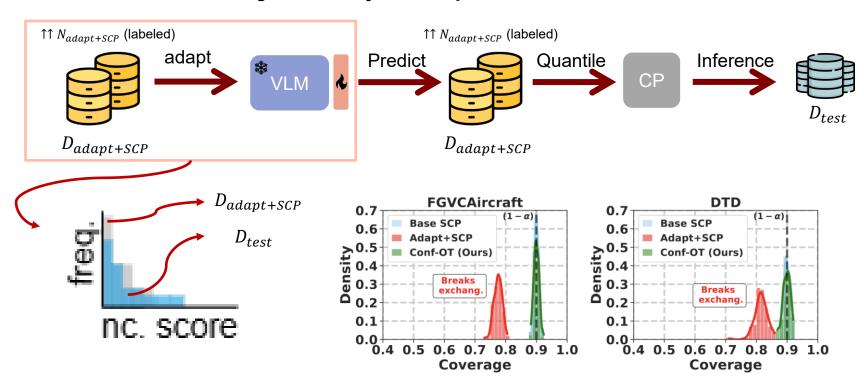
3. Modern scenario adapting foundation models.











There is life beyond vanilla split conformal predictors!!!

#### Transduction with Confidence and Credibility

C. Saunders, A. Gam merman, V. Vovk Royal Holloway, University of London Egham, Surrey, England. {craig,alex,vovk}@dcs.rhbnc.ac.nk

Saunders et al. Transduction with Confidence and Credibility, IJCAI'99.

# Algorithmic Learning in a Random World

Vladimir Vovk University of London Egham, United Kingdom

Vovk et al. Algorithmic learning in a random world, Springer'05.

$$\underbrace{(\mathbf{x}_1, y_1), ..., (\mathbf{x}_i, y_i), ..., (\mathbf{x}_N, y_N)}_{\mathcal{D}_{train}}, (\mathbf{x}_{N+1}, ?)$$

$$\underbrace{(\mathbf{x}_1, y_1), ..., (\mathbf{x}_i, y_i), ..., (\mathbf{x}_N, y_N)}_{\mathcal{D}_{train}}, (\mathbf{x}_{N+1}, ?)$$

- 1) We know that, for a **test sample**, the **true label** of a test point lies **somewhere on the label space**.
- 2) Let's **fit the model wich each label assignment** and check if the **errors** on the test point **conform** to the training observations.

#### A: For each test data point...

$$(\mathbf{x}_1, y_1), ..., (\mathbf{x}_i, y_i), ..., (\mathbf{x}_N, y_N), (\mathbf{x}_{N+1}, ?)$$

B: For each label...

$$(\mathbf{x}_1, y_1), ..., (\mathbf{x}_i, y_i), ..., (\mathbf{x}_N, y_N), (\mathbf{x}_{N+1}, y)$$

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B: For each label...

$$(\mathbf{x}_1, y_1), ..., (\mathbf{x}_i, y_i), ..., (\mathbf{x}_N, y_N), (\mathbf{x}_{N+1}, y)$$

1. Train model on joint dataset

$$\pi(\cdot)^y$$
:  $y_{N+1} = y \in \mathcal{Y}$ 

#### A: For each test data point...

$$(\mathbf{x}_1, y_1), ..., (\mathbf{x}_i, y_i), ..., (\mathbf{x}_N, y_N), (\mathbf{x}_{N+1}, ?)$$

B: For each label...

$$(\mathbf{x}_1, y_1), ..., (\mathbf{x}_i, y_i), ..., (\mathbf{x}_N, y_N), (\mathbf{x}_{N+1}, y)$$

1. Train model on joint dataset

$$\pi(\cdot)^y: y_{N+1}=y\in\mathcal{Y}$$

2. Search quantile in training data

$$s_i^y = \mathcal{S}(\pi_i^y(\mathbf{x}), y_i)$$

3. Accept/Reject label

$$\mathcal{C}(\mathbf{x}) = \{ y \in \mathcal{Y} : s^y \le \hat{s}^y \}$$

#### A: For each test data point...

$$(\mathbf{x}_1, y_1), ..., (\mathbf{x}_i, y_i), ..., (\mathbf{x}_N, y_N), (\mathbf{x}_{N+1}, ?)$$

B: For each label...

$$(\mathbf{x}_1, y_1), ..., (\mathbf{x}_i, y_i), ..., (\mathbf{x}_N, y_N), (\mathbf{x}_{N+1}, y)$$

1. Train model on joint dataset

$$\pi(\cdot)^y: y_{N+1} = y \in \mathcal{Y}$$

Training a model for each test sample and label combination. Computationally unfeasible

# **Full Conformal Adaptation (FCA)**

A: For each test data point...

$$(\mathbf{v}_1,y_1),...,(\mathbf{v}_i,y_i),...,(\mathbf{v}_N,y_N),(\mathbf{v_{N+1}}?)$$

B: For each label...

$$(\mathbf{v}_1, y_1), ..., (\mathbf{v}_i, y_i), ..., (\mathbf{v}_N, y_N), (\mathbf{v}_{N+1}, y)$$

1. Adapt the model on joint dataset

$$p(\mathbf{W}^*, \cdot)^y$$
 :  $y_{N+1} = y \in \mathcal{Y}$ 

Leveraging efficient linear probing solvers, the adaptation phase takes few milliseconds

# **Full Conformal Adaptation (FCA)**

#### A: For each test data point...

$$(\mathbf{v}_1, y_1), ..., (\mathbf{v}_i, y_i), ..., (\mathbf{v}_N, y_N), (\mathbf{v}_{N+1}, ?)$$

B: For each label...

$$(\mathbf{v}_1, y_1), ..., (\mathbf{v}_i, y_i), ..., (\mathbf{v}_N, y_N), (\mathbf{v}_{N+1}, y)$$

1. Adapt the model on joint dataset

$$p(\mathbf{W}^*,\cdot)^y:y_{N+1}=y\in\mathcal{Y}$$

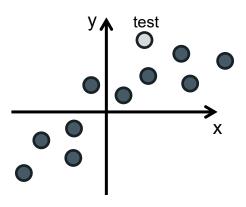
2. Search quantile in training data

$$s_i^y = \mathcal{S}(p(\mathbf{W}^*, \mathbf{v}_i)^y \ y_i)$$

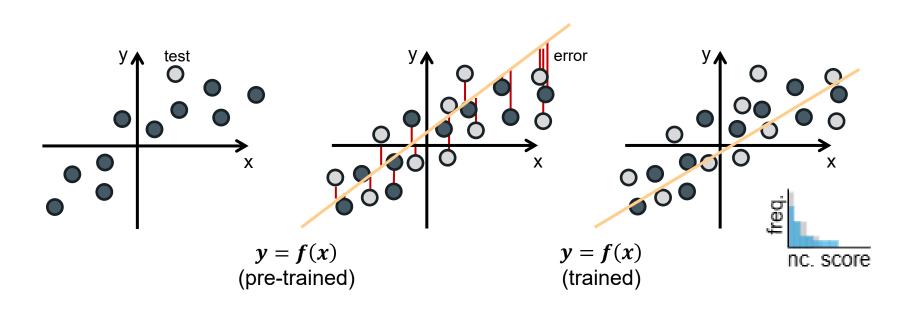
3. Accept/Reject label

$$\mathcal{C}(\mathbf{x}) = \{ y \in \mathcal{Y} : s^y \le \hat{s}^y \}$$

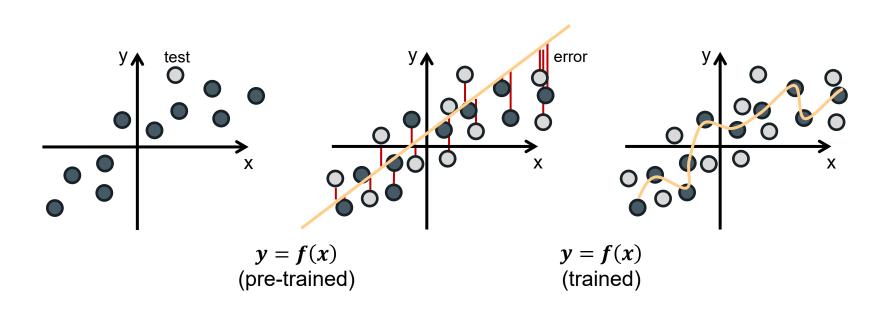
Interpretation: Why does it work?



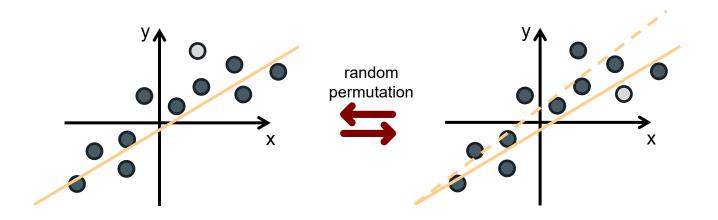
Interpretation: Why does it work?



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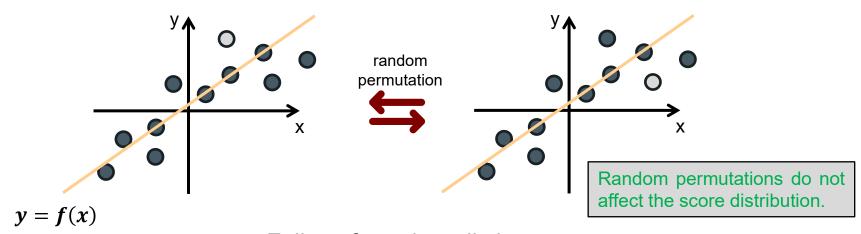


A fast trick to check exchangeability of the pipeline



Adapt + Split Conformal Prediction

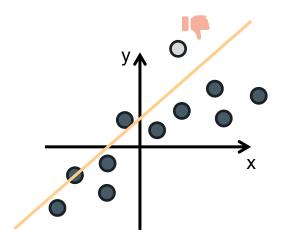
A fast trick to check exchangeability of the pipeline



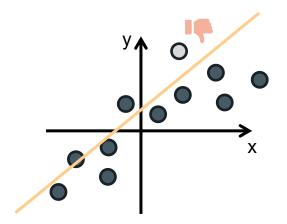
Full conformal prediction

The model is trained using the test point:

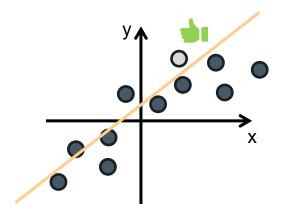
$$(\mathbf{v}_1, y_1), ..., (\mathbf{v}_i, y_i), ..., (\mathbf{v}_N, y_N), (\mathbf{v}_{N+1}, y)$$



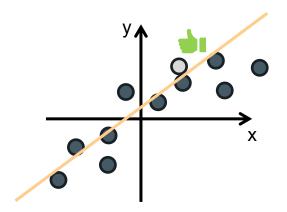
Full conformal prediction



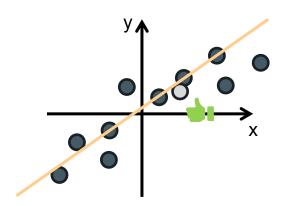
Full conformal prediction



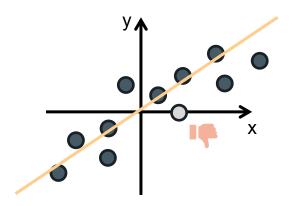
Full conformal prediction



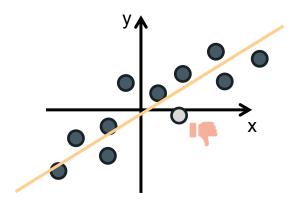
Full conformal prediction



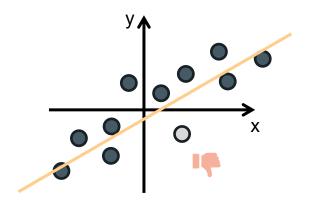
Full conformal prediction



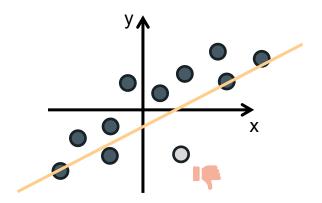
Full conformal prediction



Full conformal prediction

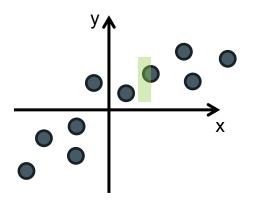


Full conformal prediction



Full conformal prediction

Full conformal prediction loop



# **Full Conformal Adaptation (FCA)**

Method		$\alpha = 0.10$		
2.2001100	$\mathrm{ACA}\!\!\uparrow$	Cov.	$\mathrm{Size}\!\!\downarrow$	$CCV\downarrow$
O SCP	50.2	0.890	3.99	9.96
$egin{array}{c} egin{array}{c} \operatorname{Adapt+SCP} \\ \operatorname{FCA}\ (Ours) \end{array}$	$67.1_{+16.9}$	0.842	$2.40_{-1.59}$	$11.17_{\pm 1.21}$
FCA (Ours)	$67.1_{+16.9}$	0.896	$2.91_{\text{-}1.08}$	8.38-1.58
Method		$\alpha = 0.05$		
2.2231104	$ACA\uparrow$	Cov.	Size↓	$CCV\downarrow$

Average performance across tasks (from 4 until 20 categories, 8 in average)

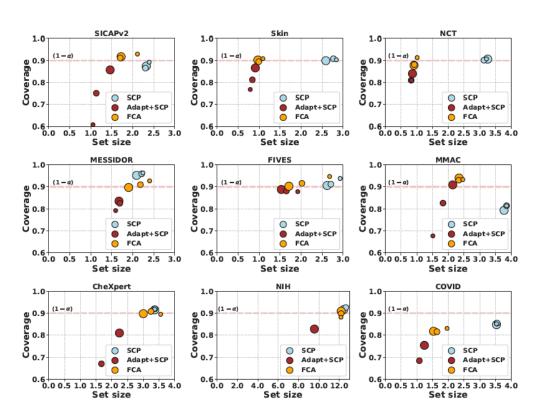
Adapt+SCP **67.1**<sub>+16.9</sub> 0.921 **3.07**<sub>-1.81</sub> 6.87<sub>+1.19</sub>

FCA (Ours) 67.1<sub>+16.9</sub> 0.952 3.56<sub>-1.32</sub> 5.02<sub>-0.66</sub>

0.951

50.2

 ${\rm co}_{\rm SCP}$ 



4.88

5.68

# What about non-conformity scores?

$$S_{LAC}(\mathbf{x}, y) = 1 - p_{k=y}$$

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

$$S_{APS}(\mathbf{x}, y) = \rho_x(y) + p_{k=y} \cdot u$$

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

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

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

# What about non-conformity scores?

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∞ SCP	50.2			9.59	
Adapt+SCP	$67.1_{+16.9}$	0.858	$2.56_{-1.49}$	$8.57_{-1.02}$	
$\stackrel{\mathbf{d}}{FCA} \stackrel{\mathrm{Adapt+SCP}}{\mathrm{FCA}}$	$67.1_{+16.9}$	0.898	$3.06_{-0.99}$	$6.12_{-3.47}$	
SCP	50.2	0.901	4.16	9.55	
Adapt+SCP	$67.1_{+16.9}$	0.856	$\boldsymbol{2.55_{-1.61}}$	$8.64_{-0.91}$	
$ \overset{\mathbf{C}}{\overset{\mathbf{CP}}}{\overset{\mathbf{CP}}{\overset{\mathbf{CP}}{\overset{\mathbf{CP}}{\overset{\mathbf{CP}}{\overset{\mathbf{CP}}{\overset{\mathbf{CP}}{\overset{\mathbf{CP}}}{\overset{\mathbf{CP}}{\overset{\mathbf{CP}}{\overset{\mathbf{CP}}{\overset{\mathbf{CP}}{\overset{\mathbf{CP}}}{\overset{\mathbf{CP}}{\overset{\mathbf{CP}}{\overset{\mathbf{CP}}}{\overset{\mathbf{CP}}{\overset{\mathbf{CP}}}{\overset{\mathbf{CP}}{\overset{\mathbf{CP}}}{\overset{\mathbf{CP}}{\overset{\mathbf{CP}}}{\overset{\mathbf{CP}}}{\overset{\mathbf{CP}}}{\overset{\mathbf{CP}}}}{\overset{\mathbf{CP}}}{\overset{\mathbf{CP}}}{\overset{\mathbf{CP}}{\overset{\mathbf{CP}}{\overset{\mathbf{CP}}{\overset{\mathbf{CP}}{\overset{\mathbf{CP}}}{\overset{\mathbf{CP}}{\overset{\mathbf{CP}}}{\overset{\mathbf{CP}}}{\overset{\mathbf{CP}}}{\overset{\mathbf{CP}}}}}{\overset{\mathbf{CP}}}{\overset{\mathbf{CP}}}{\overset{\mathbf{CP}}}{\overset{\mathbf{CP}}}{\overset{\mathbf{CP}}}}{\overset{\mathbf{CP}}}}{\overset{\mathbf{CP}}}}{\overset{\mathbf{CP}}}{\overset{\mathbf{CP}}}{\overset{\mathbf{CP}}}{\overset{\mathbf{CP}}}}{\overset{\mathbf{CP}}}}{\overset{\mathbf{CP}}}}{\overset{\mathbf{CP}}}{\overset{\mathbf{CP}}}{\overset{\mathbf{CP}}}}{\overset{\mathbf{CP}}}}{\overset{\mathbf{CP}}}}{\overset{\mathbf{CP}}}}{\overset{\mathbf{CP}}}}{\overset{\mathbf{CP}}}}{\overset{\mathbf{CP}}}}{\overset{\mathbf{CP}}}}{\overset{\mathbf{CP}}}}{\overset{\mathbf{CP}}}}{\overset{\mathbf{CP}}}}{\overset{\mathbf{CP}}}}{\overset{\mathbf{CP}}}{\overset{\mathbf{CP}}}}{\overset{\mathbf{CP}}}}{\overset{\mathbf{CP}}}}}{\overset{\mathbf{CP}}}{\overset{\mathbf{CP}}}}{\overset{\mathbf{CP}}}}{\overset{\mathbf{CP}}}}{\overset{\mathbf{CP}}}}{\overset{\mathbf{CP}}}}{\overset{\mathbf{CP}}}}{\overset{\mathbf{CP}}}}{\overset{\mathbf{CP}}}}{\overset{\mathbf{CP}}}}{\overset{\mathbf{CP}}}}{\overset{\mathbf{CP}}}}{$	$67.1_{+16.9}$	0.898	$3.05_{\text{-}1.11}$	$6.21_{-3.34}$	

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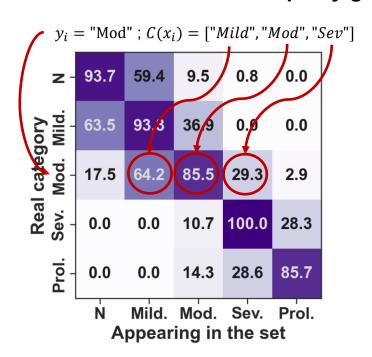
$$S_{\text{RAPS}}(\mathbf{x}, y) = S_{\text{APS}}(\mathbf{x}, y) + \lambda \cdot (o(\mathbf{x}, y) - k_{\text{reg}})^+$$

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_						
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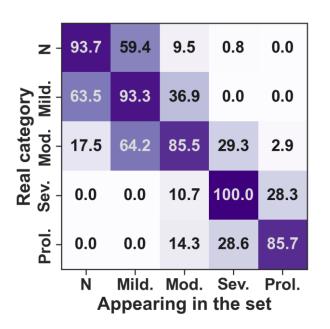
# Interpretability of conformal sets

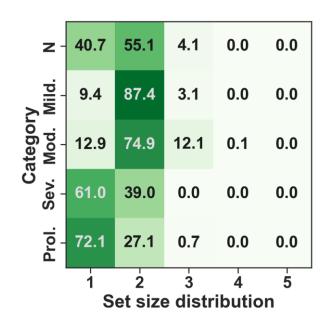
Use-case: diabetic retinopathy grading. Top-1 accuracy: 71%; Coverage: 90%.

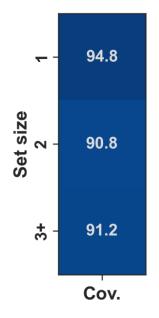


# Interpretability of conformal sets

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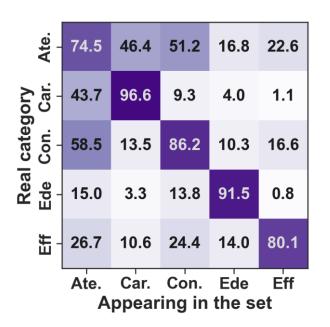


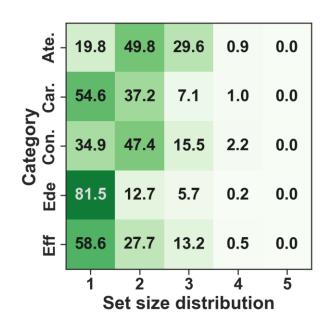


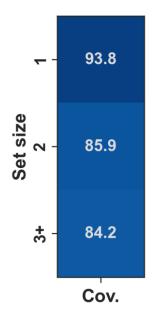


# Interpretability of conformal sets

Use-case: chest X-ray findings classification. Top-1 accuracy: 81%; Coverage: 90%.

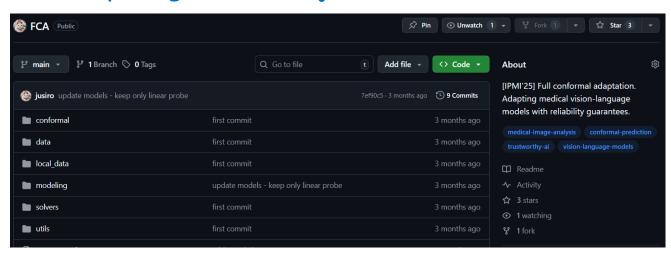






# Implementation & benchmark publicly available

# https://github.com/jusiro/FCA





# Implementation & benchmark publicly available

https://github.com/jusiro/FCA/blob/main/docs/awesome-miccai-conformal.md



