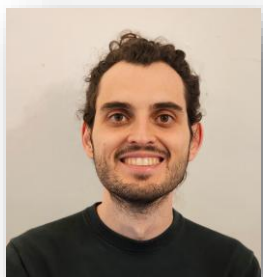


Full Conformal Adaptation of Medical Vision-Language Models

Julio
Silva-Rodríguez



Leo
Fillioux



Paul-Henry
Cournède



Maria
Vakalopoulou



Stergios
Christodoulidis



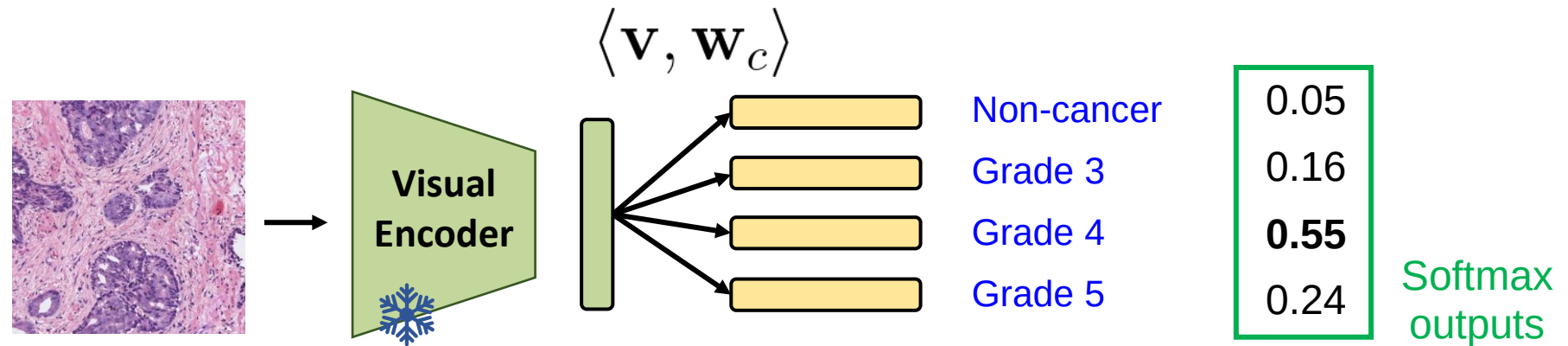
Ismail
Ben Ayed



Jose
Dolz



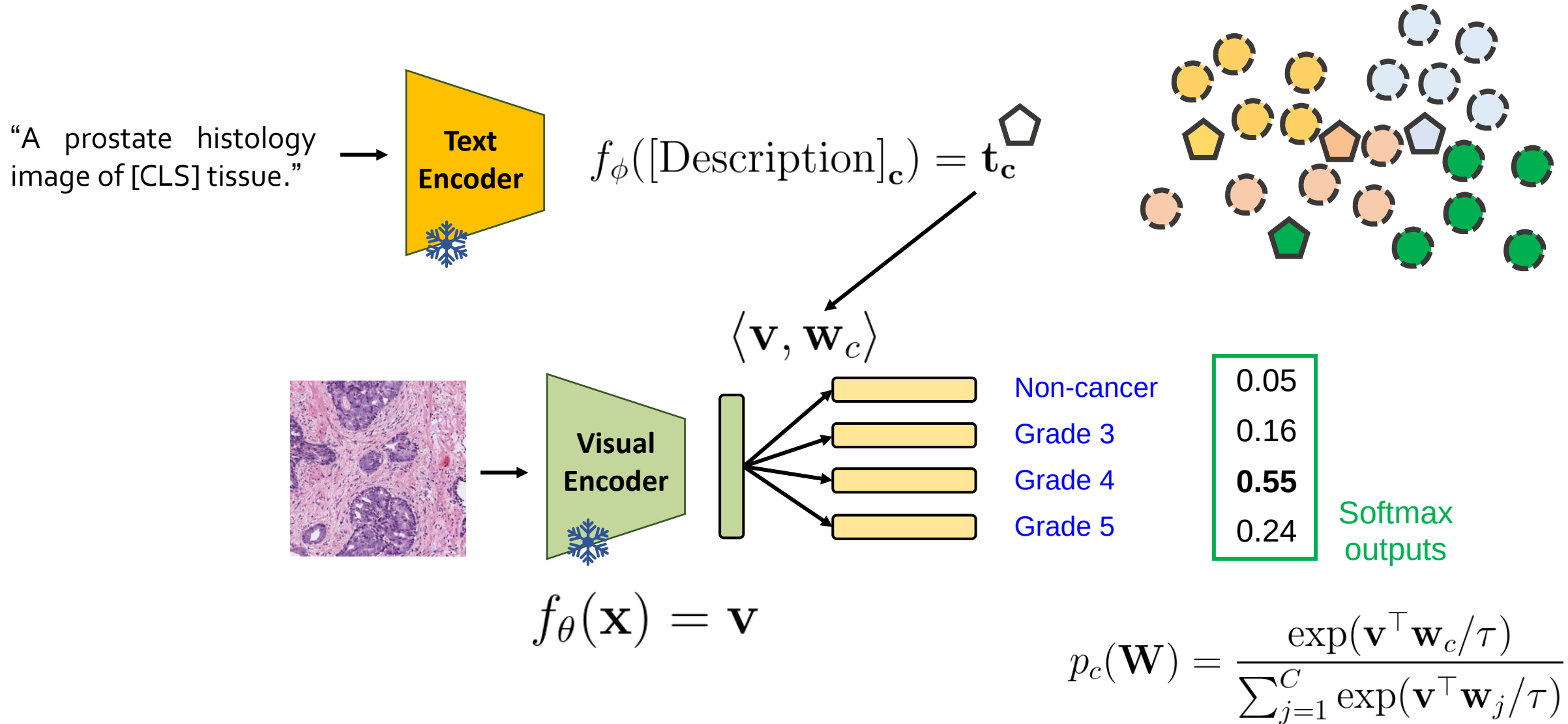
Vision-Language Models



$$f_{\theta}(\mathbf{x}) = \mathbf{v}$$

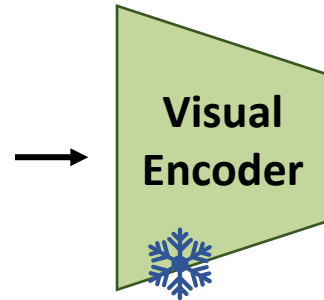
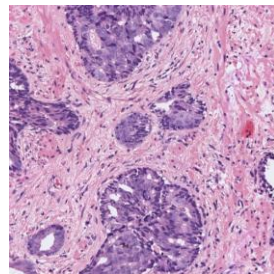
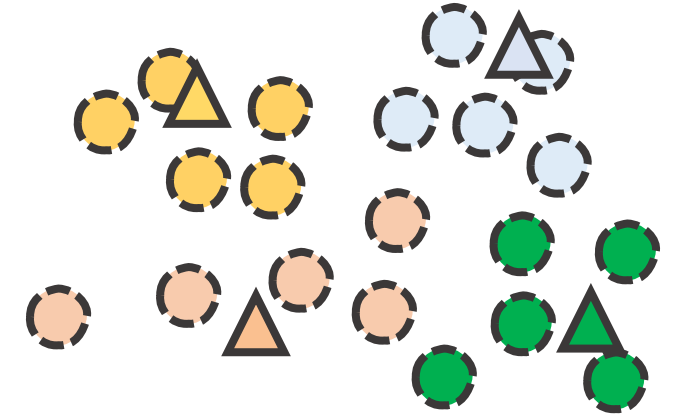
$$p_c(\mathbf{W}) = \frac{\exp(\mathbf{v}^{\top} \mathbf{w}_c / \tau)}{\sum_{j=1}^C \exp(\mathbf{v}^{\top} \mathbf{w}_j / \tau)}$$

Vision-Language Models

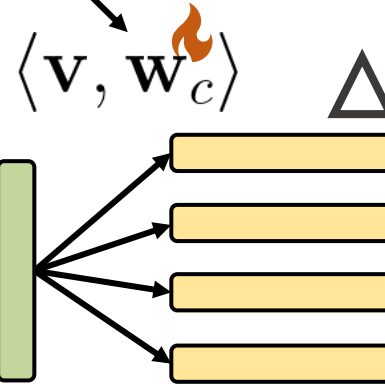


Vision-Language Models

Support set
(labeled few-shot)
 $N = K \text{ (shots)} \times C \text{ (classes)}$



$$f_{\theta}(\mathbf{x}) = \mathbf{v}$$



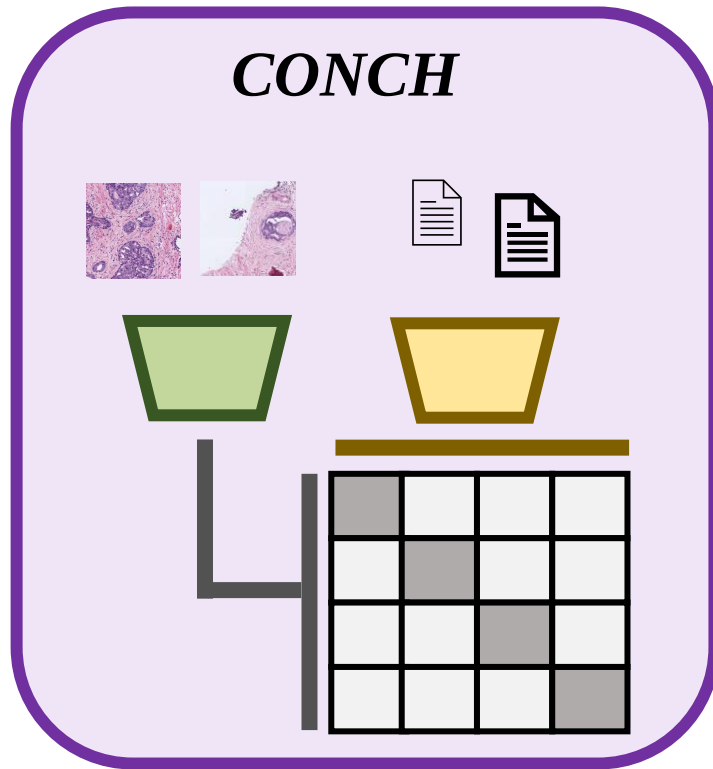
Non-cancer
Grade 3
Grade 4
Grade 5

0.05
0.16
0.55
0.24

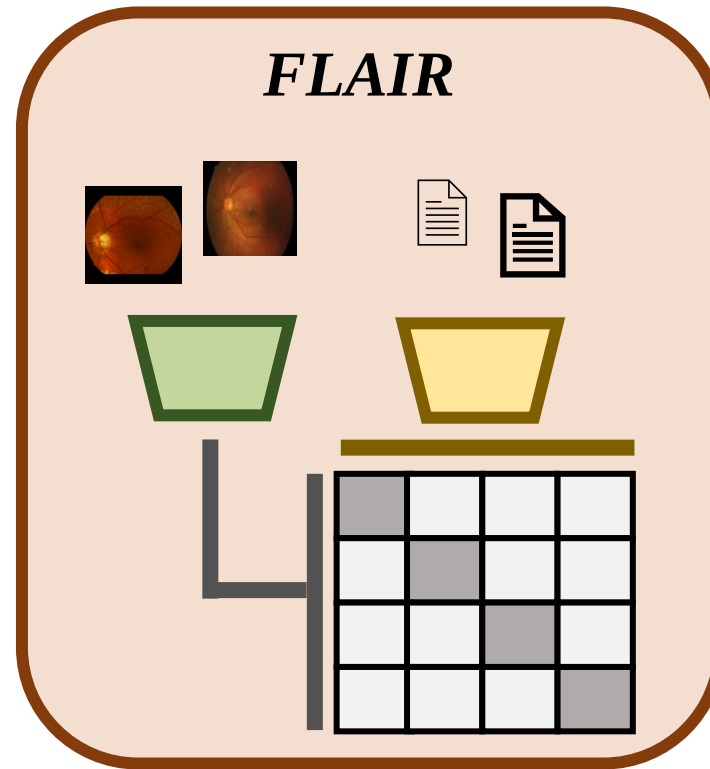
Softmax
outputs

$$p_c(\mathbf{W}) = \frac{\exp(\mathbf{v}^{\top} \mathbf{w}_c / \tau)}{\sum_{j=1}^C \exp(\mathbf{v}^{\top} \mathbf{w}_j / \tau)}$$

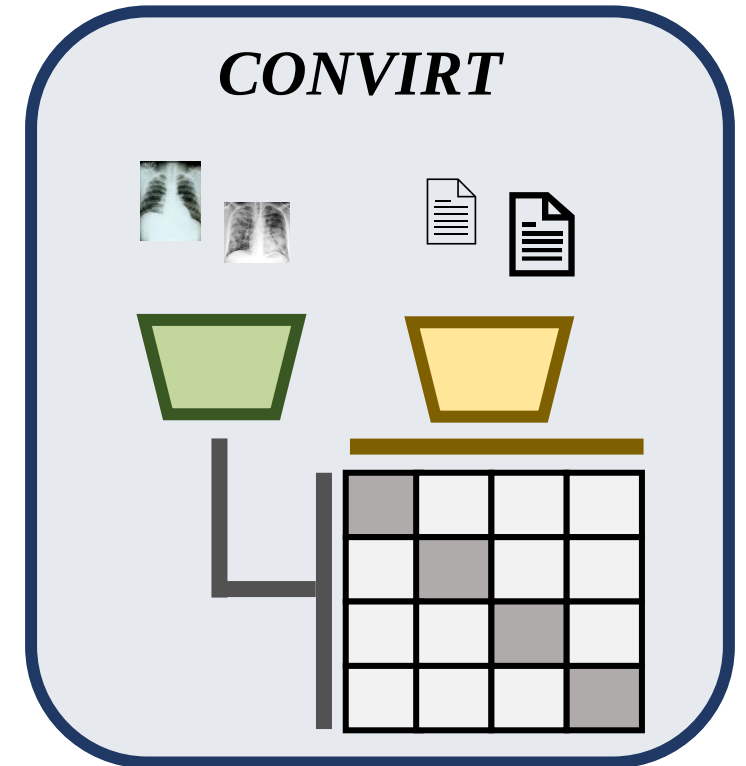
Medical Vision-Language Models



Histology



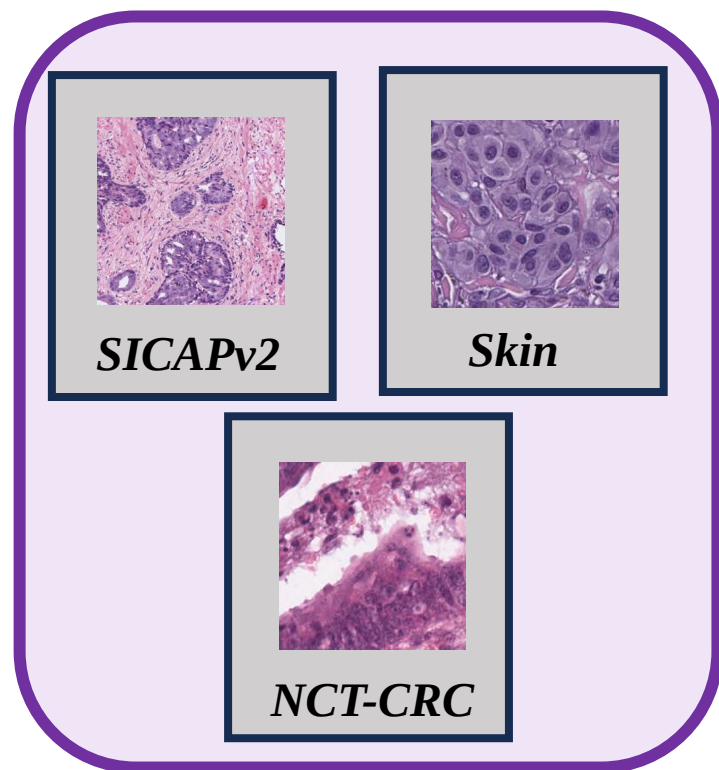
Ophthalmology



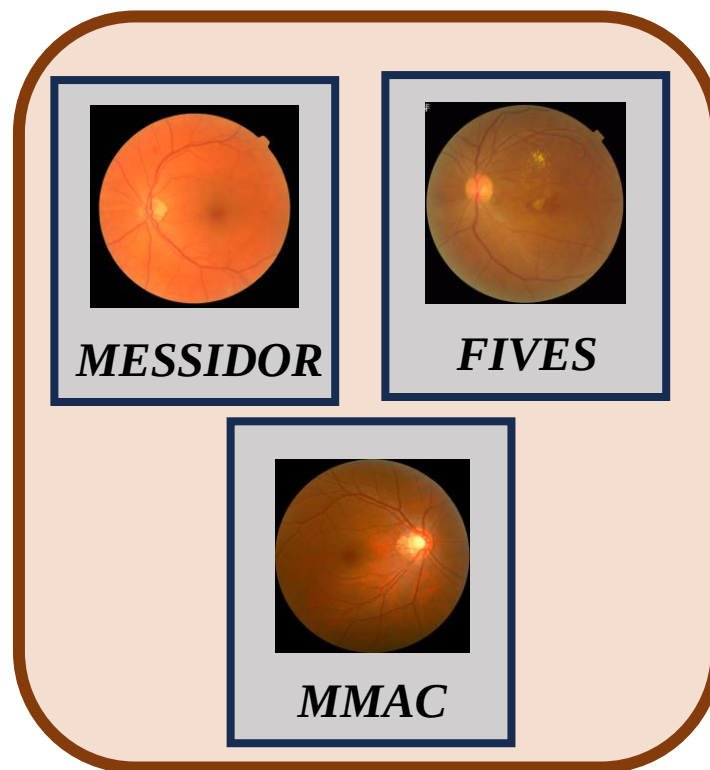
Chest X-ray

Medical Vision-Language Models

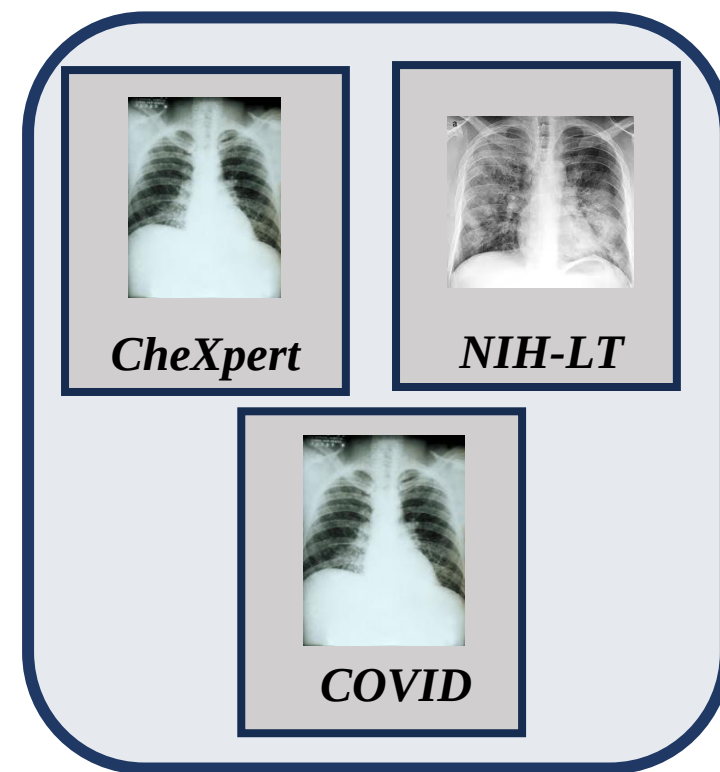
■ Downstream tasks



Histology



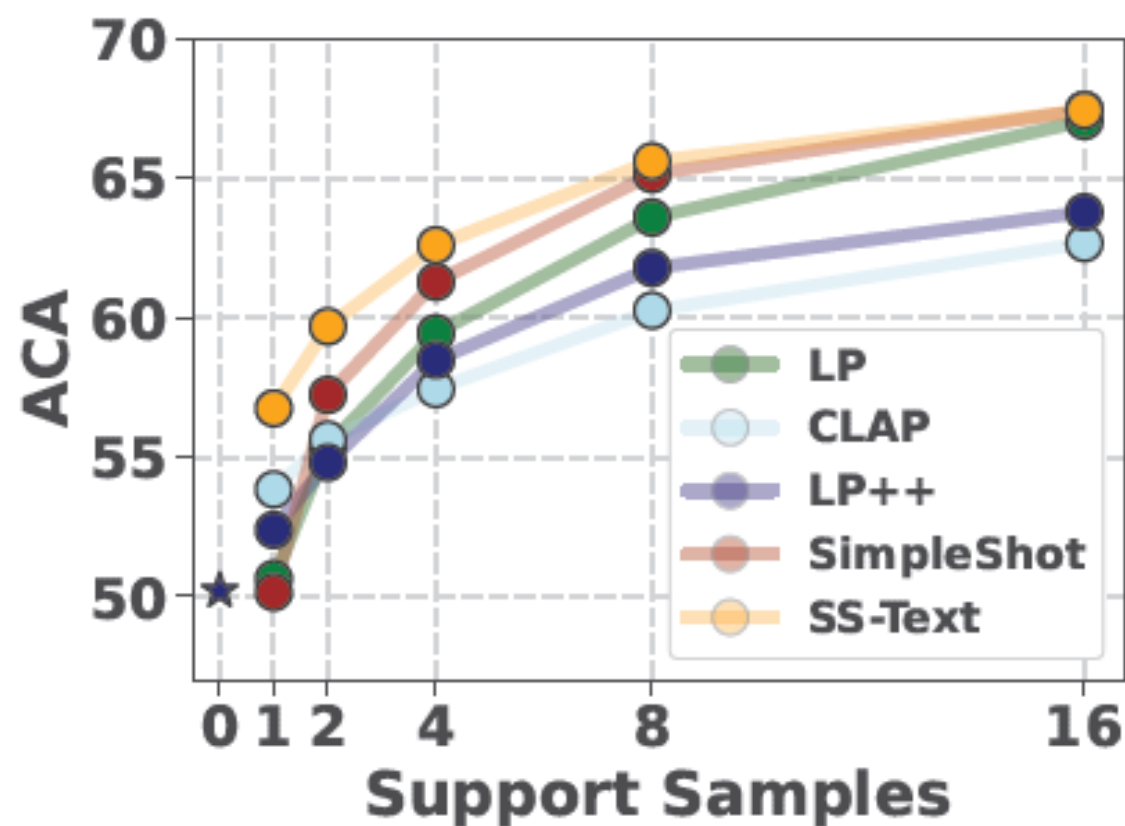
Ophtalmology



Chest X-ray

Medical Vision-Language Models

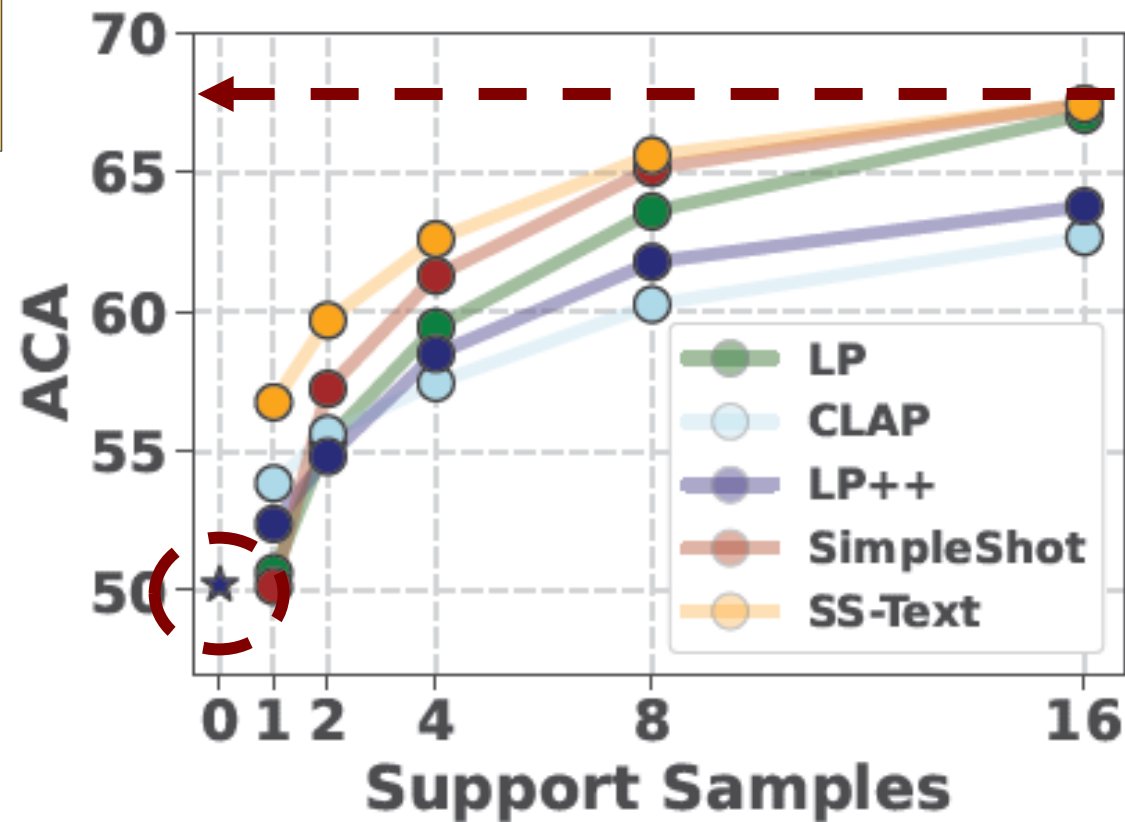
- Efficient downstream adaptation



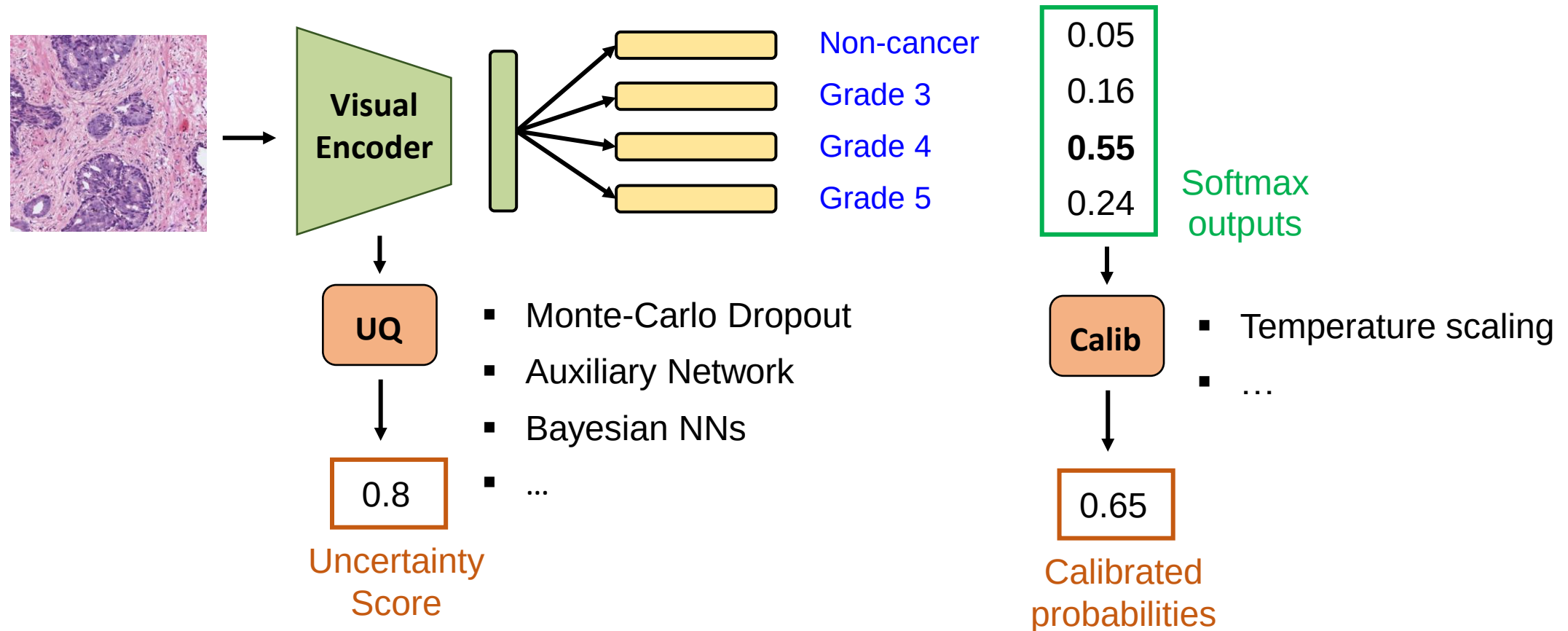
Medical Vision-Language Models

- Efficient downstream adaptation

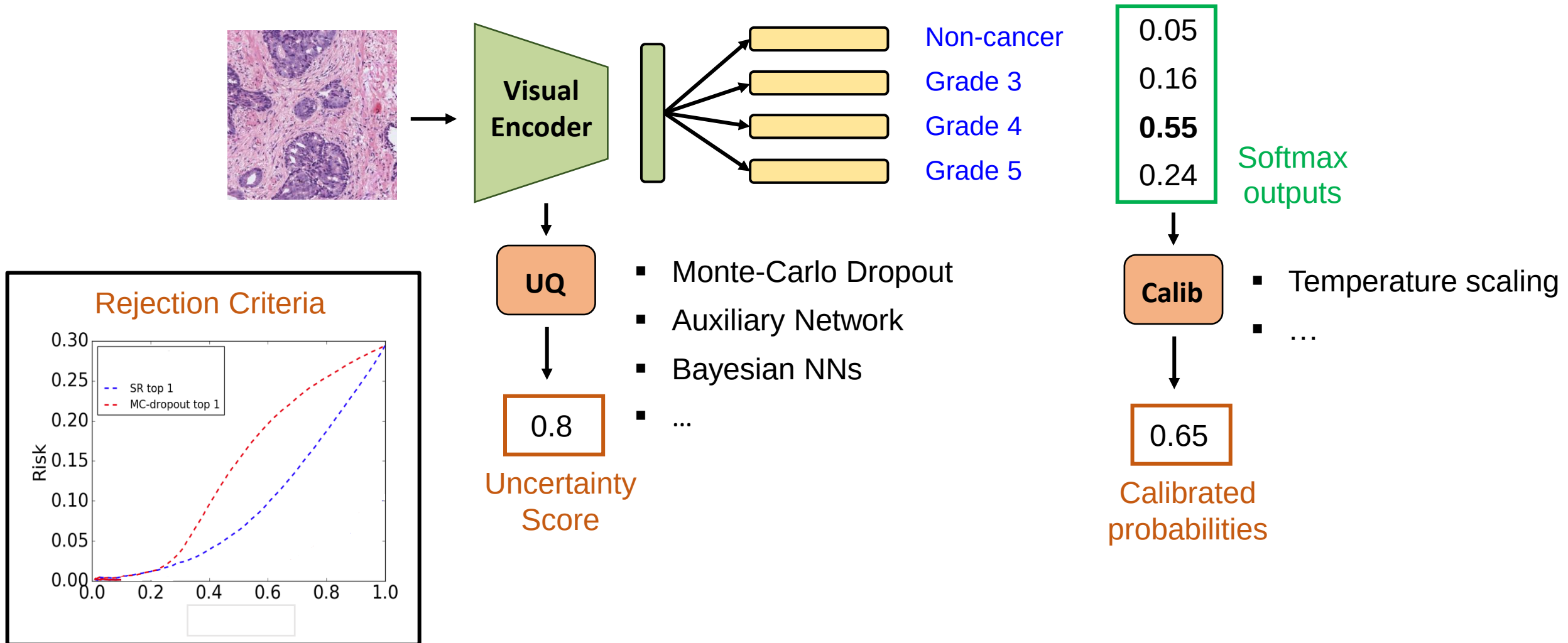
Machine learning models fail!



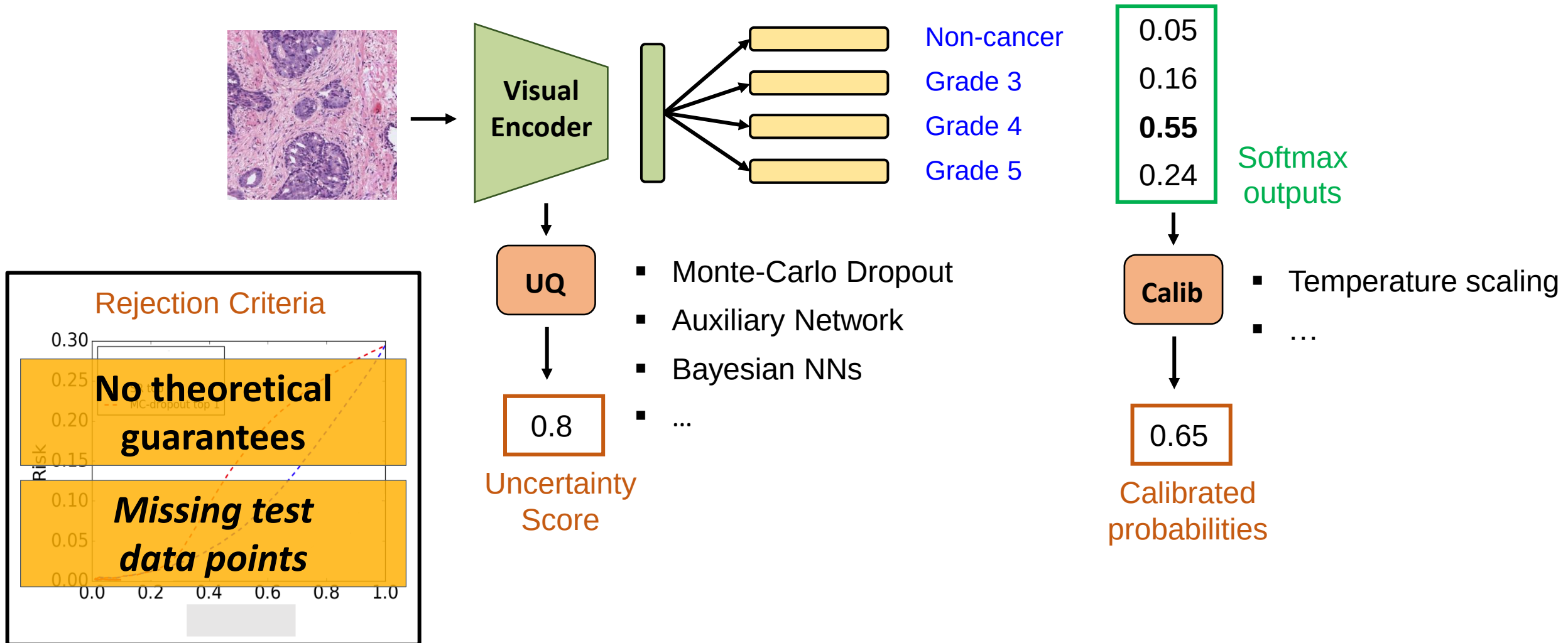
Uncertainty quantification through sample rejection



Uncertainty quantification through sample rejection



Uncertainty quantification through sample rejection



Split Conformal Prediction

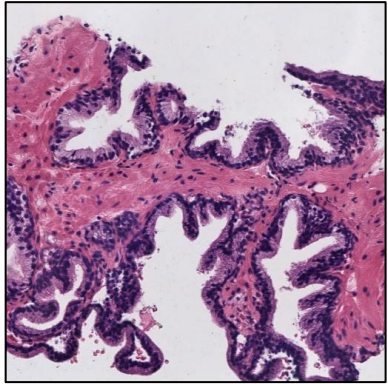
$$\mathcal{P}(Y \in C(\mathbf{x})) \geq 1 - \alpha$$

Split Conformal Prediction

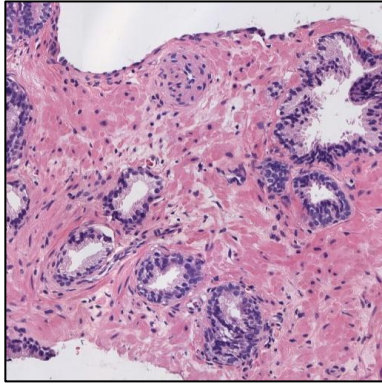
$$\mathcal{P}(Y \in C(\mathbf{x})) \geq 1 - \alpha$$

Conformal sets

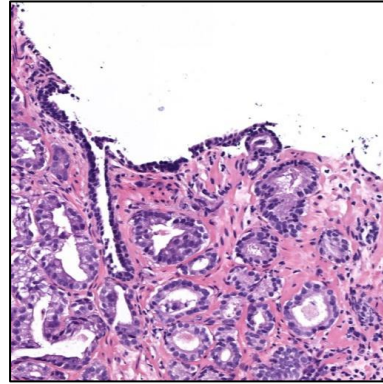
Error rate, e.g., 10%



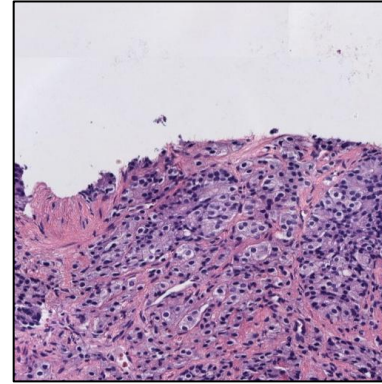
GT: NC
CP: [NC]



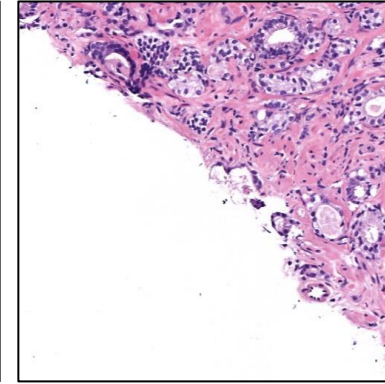
GT: G3
CP: [G3]



GT: G3
CP: [G3, G4]



GT: G5
CP: [G5]



GT: G5
CP: [G4, G5]

Split Conformal Prediction

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

■ How to construct $C(\mathbf{x})$?

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

non-conformity score



Calibration set
(labeled few-shot)



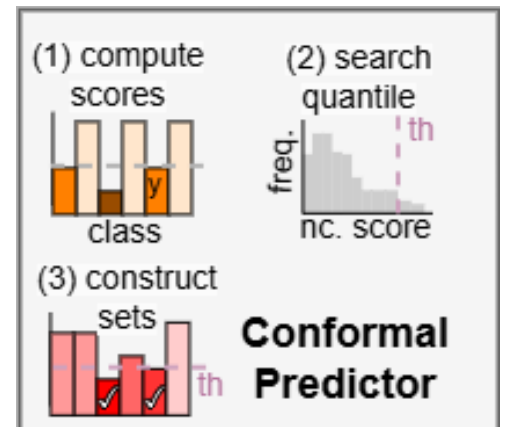
$$\hat{s} = \inf \left[s : \frac{|\{i \in \{1, \dots, N\} : s_i \leq s\}|}{N} \geq \frac{\lceil (N+1)(1-\alpha) \rceil}{N} \right]$$



Test set
(unlabeled)



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



Split Conformal Prediction

Marginal over $\mathcal{X}\mathcal{Y}$

Under cal/test exchangeability

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

■ How to construct $C(\mathbf{x})$?

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

non-conformity score



Calibration set
(labeled few-shot)



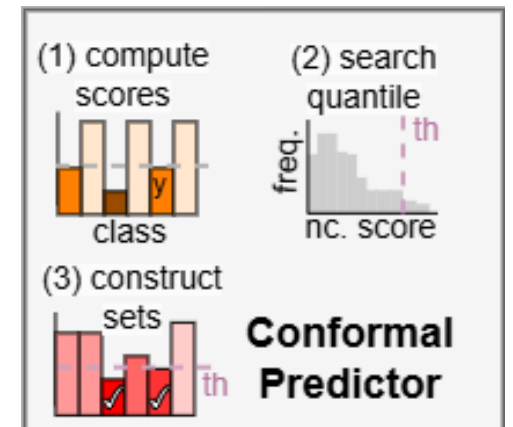
$$\hat{s} = \inf \left[s : \frac{|\{i \in \{1, \dots, N\} : s_i \leq s\}|}{N} \geq \frac{\lceil (N+1)(1-\alpha) \rceil}{N} \right]$$



Test set
(unlabeled)

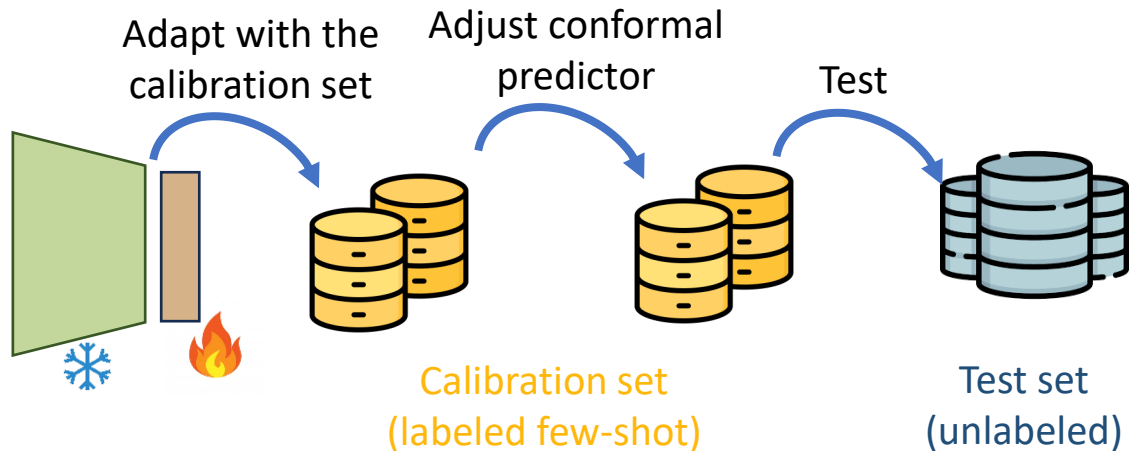


$$C(\mathbf{x}) = \{y \in \mathcal{Y} : \mathcal{S}(\mathbf{x}, y) \leq \hat{s}\}$$



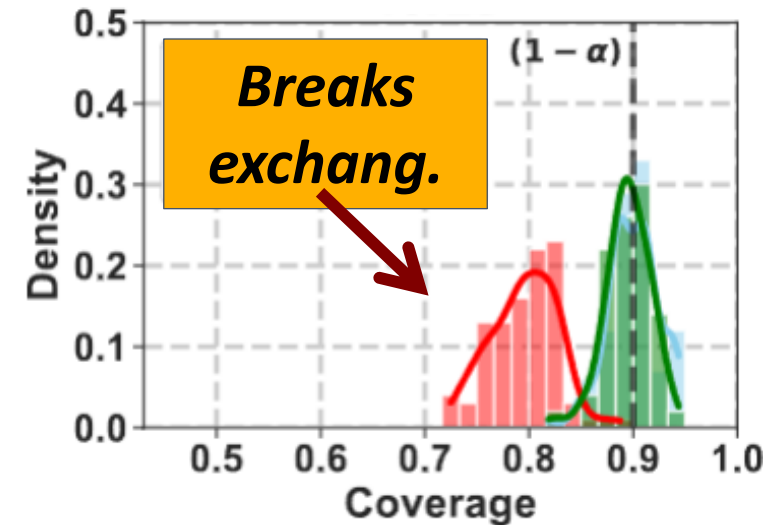
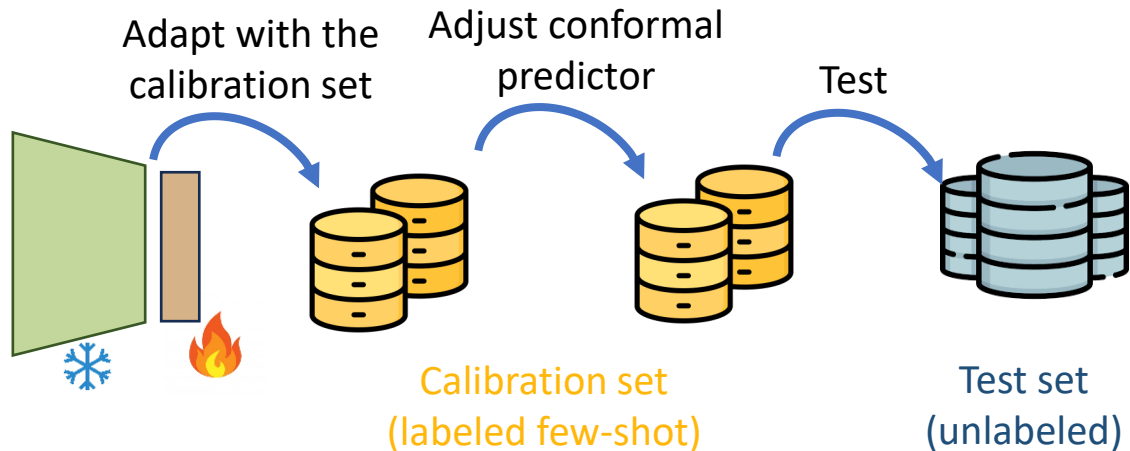
Pitfalls of conformal prediction and transfer learning

- Can we adapt and conformalize with the same calibration data?



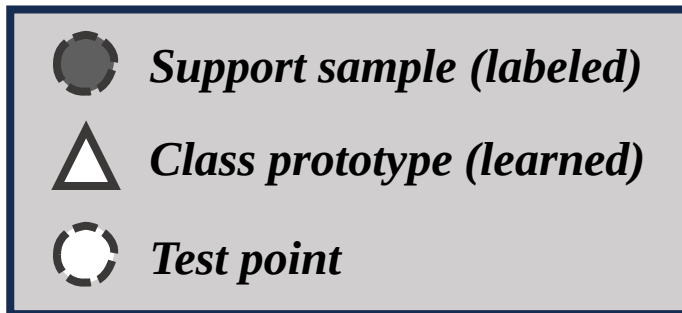
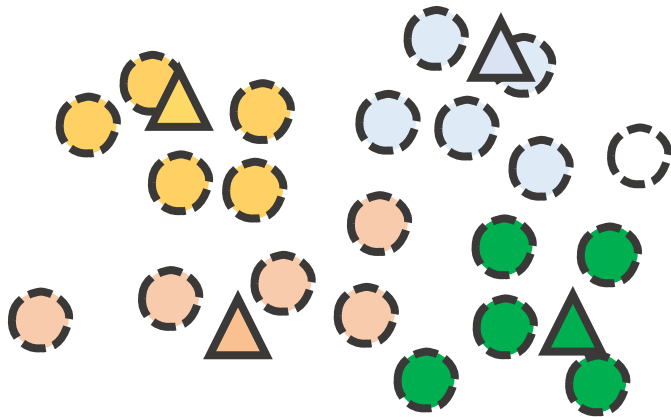
Pitfalls of conformal prediction and transfer learning

- Can we adapt and conformalize with the same calibration data?



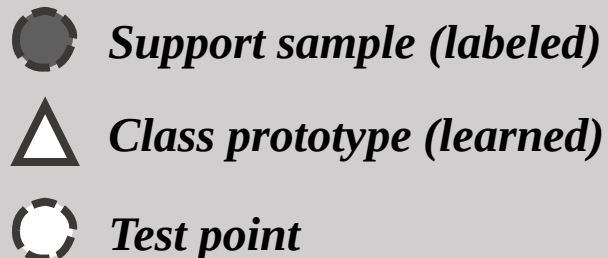
Pitfalls of conformal prediction and transfer learning

- **Why do we break the exchangeability assumption in the scores?**



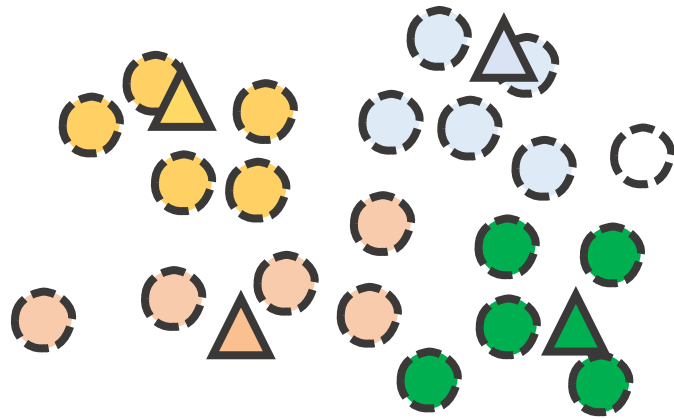
Pitfalls of conformal prediction and transfer learning

- Why do we break the exchangeability assumption in the scores?

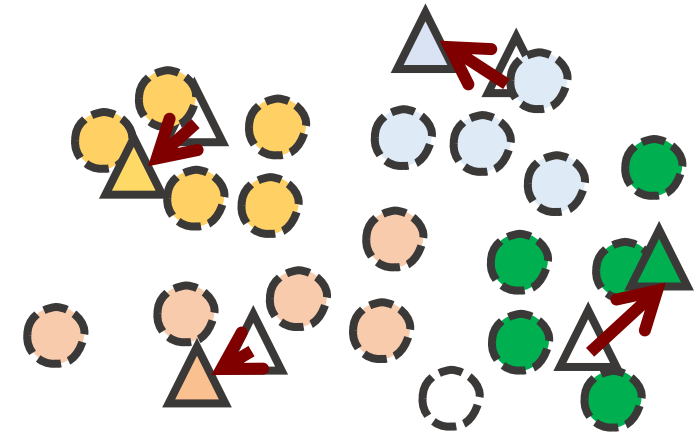


Pitfalls of conformal prediction and transfer learning

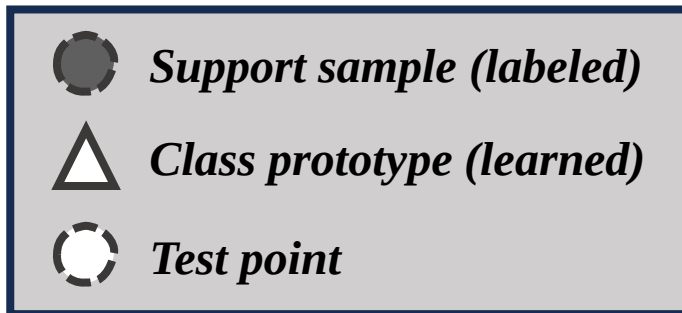
- Why do we break the exchangeability assumption in the scores?



Exchange a train and
test point

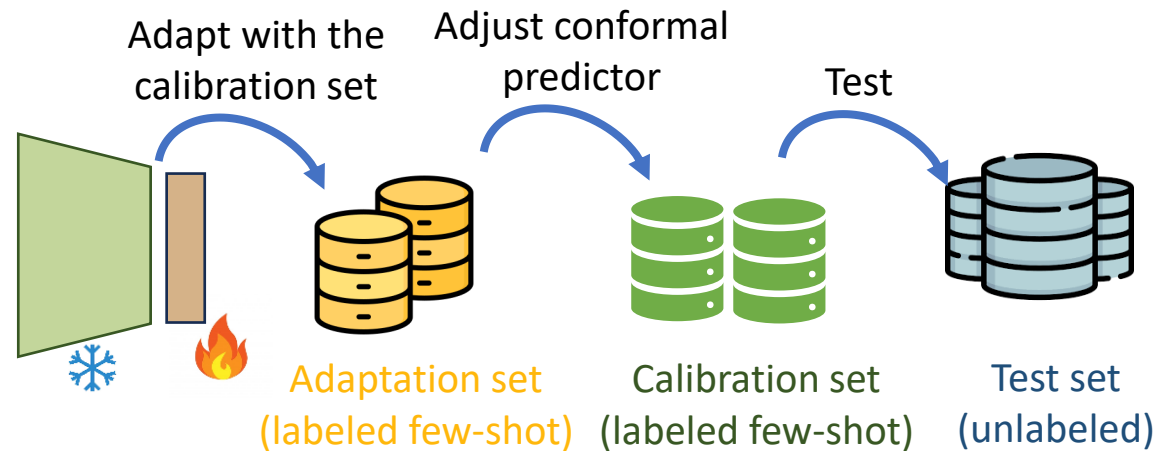


Random permutations change the
learned weights. Exchangeability
between cal/test scores is lost.



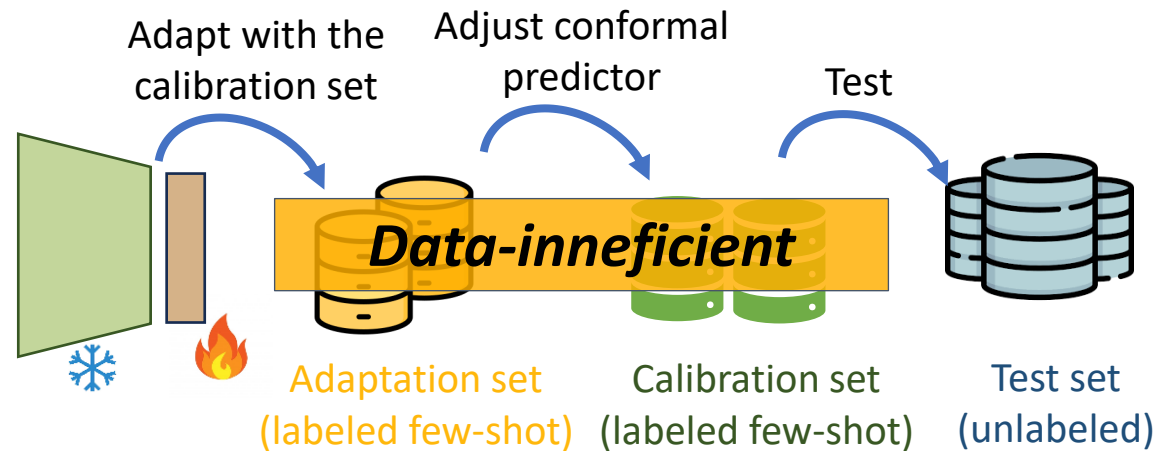
Pitfalls of conformal prediction and transfer learning

- **Alternative: adding additional data for calibration after adaptation.**



Pitfalls of conformal prediction and transfer learning

- **Alternative: adding additional data for calibration after adaptation.**



Our setting: full conformal adaptation

- Full conformal prediction scenario (Vovk *et al.* 1998).

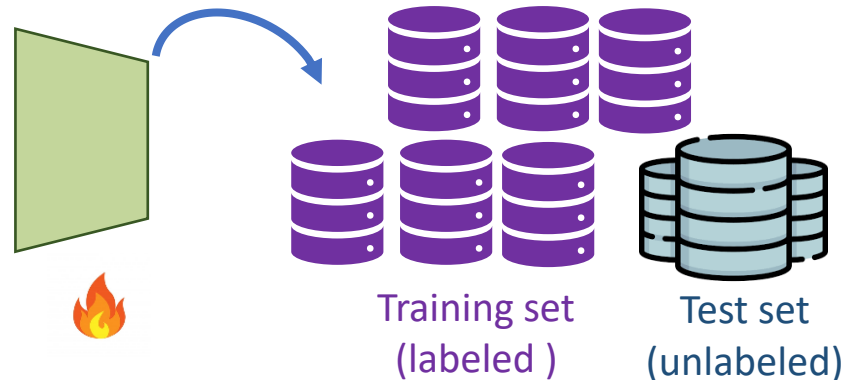
Transduction with Confidence and Credibility

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

*Algorithmic Learning
in a Random World*

Vladimir Vovk
University of London
Egham, United Kingdom

Train and conformalize
with the training + test set



Our setting: full conformal adaptation

- Full conformal prediction scenario (Vovk *et al.* 1998).

Idea:

1) We know that the true label of a test point lies on the label space.

2) Let's fit the model with each label assignment and check if the errors on the test point conform to the training observations.

Our setting: full conformal adaptation

- Full conformal prediction scenario (Vovk *et al.* 1998).

A: For each test data point...

B: For each label...

$$\mathcal{D}_{train} = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_r, y_r), \dots, (\mathbf{x}_R, y_R), (\mathbf{x}_m, y)\}$$

Our setting: full conformal adaptation

- Full conformal prediction scenario (Vovk *et al.* 1998).

A: For each test data point...

B: For each label...

$$\mathcal{D}_{train} = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_r, y_r), \dots, (\mathbf{x}_R, y_R), (\mathbf{x}_m, y)\}$$

1. Train model on joint dataset

$$(\pi(\cdot)^y): y_m = y \in \mathcal{Y}$$

Our setting: full conformal adaptation

- Full conformal prediction scenario (Vovk *et al.* 1998).

A: For each test data point...

B: For each label...

$$\mathcal{D}_{train} = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_r, y_r), \dots, (\mathbf{x}_R, y_R), (\mathbf{x}_m, y)\}$$

1. Train model on joint dataset

$$\pi(\cdot)^y : y_m = y \in \mathcal{Y}$$

2. Search quantile in training data

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

3. Accept/Reject label

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

Our setting: full conformal adaptation

- Full conformal prediction scenario (Vovk *et al.* 1998).

A: For each test data point...

B: For each label...

$$\mathcal{D}_{train} = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_r, y_r), \dots, (\mathbf{x}_R, y_R), (\mathbf{x}_m, y)\}$$

1. Train model on joint dataset

$$\pi(\cdot)^y : y_m = y \in \mathcal{Y}$$

Access to train data

2. Search quantile in training data

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

**Multiple (expensive)
model fits per sample**

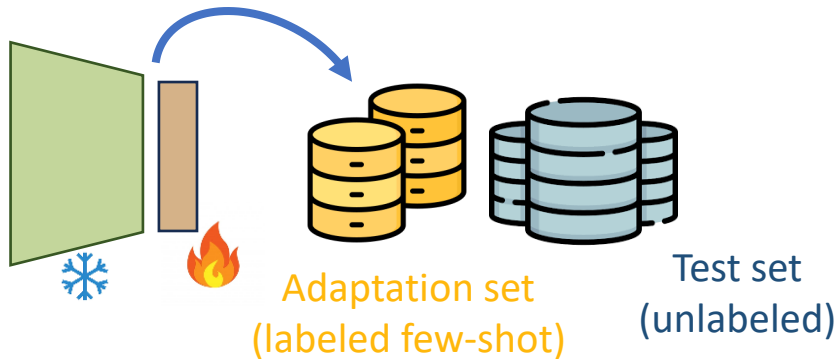
3. Accept/Reject label

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

Our setting: full conformal adaptation

- Full conformal adaptation (FCA)

Full conformal loop with the adaptation + test set



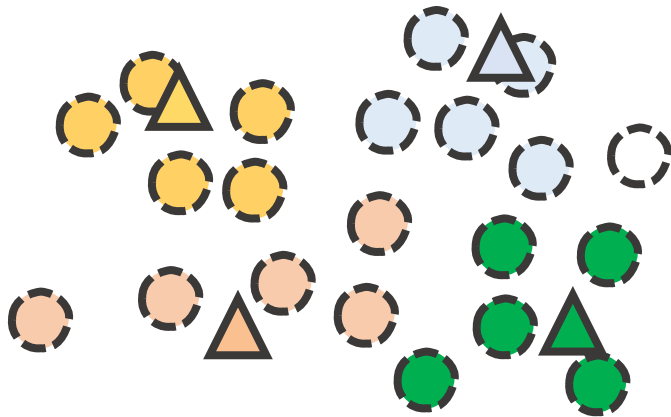
$$s_i^y = \mathcal{S}(\mathbf{p}_i(\mathbf{W}^y), y_i)$$

Access to (small) adaptation data

Múltiple (light) prototype fits per sample

Our setting: full conformal adaptation

■ Interpretation



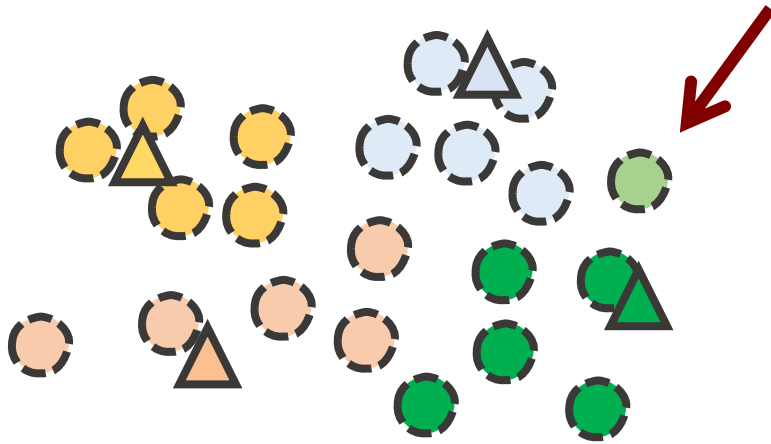
-  *Support sample (labeled)*
-  *Class prototype (learned)*
-  *Test point*

Our setting: full conformal adaptation

■ Interpretation

Assume the true label is assigned. In full conformal settings, the test point is used for training (transductive)

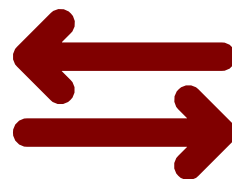
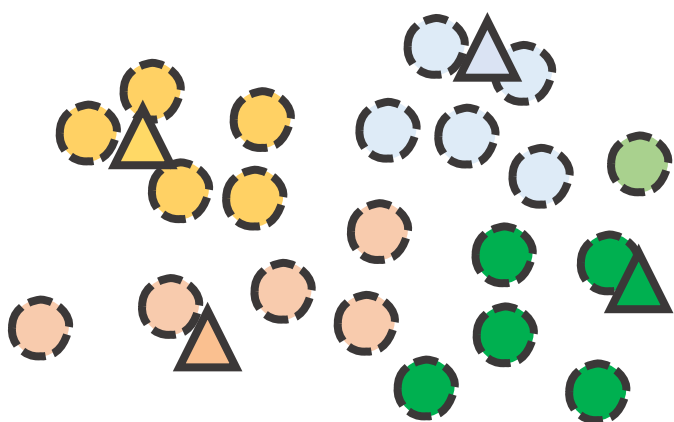
$$\mathcal{D}_{train} = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_r, y_r), \dots, (\mathbf{x}_R, y_R), (\mathbf{x}_m, y)\}$$



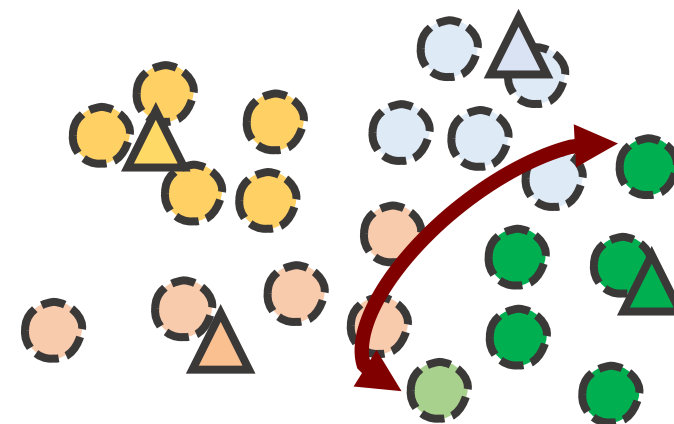
-  *Support sample (labeled)*
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Our setting: full conformal adaptation

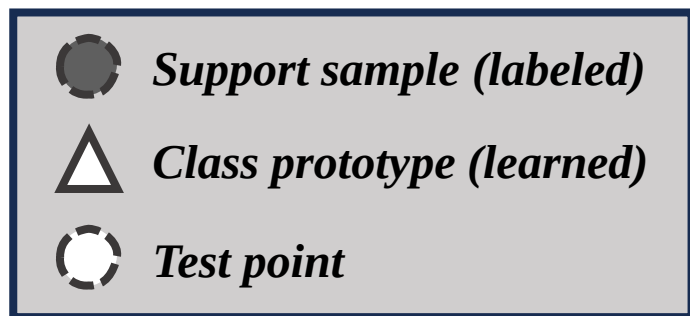
■ Interpretation



Exchange a train and
test point

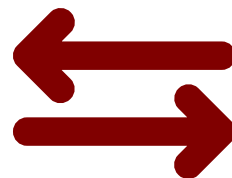
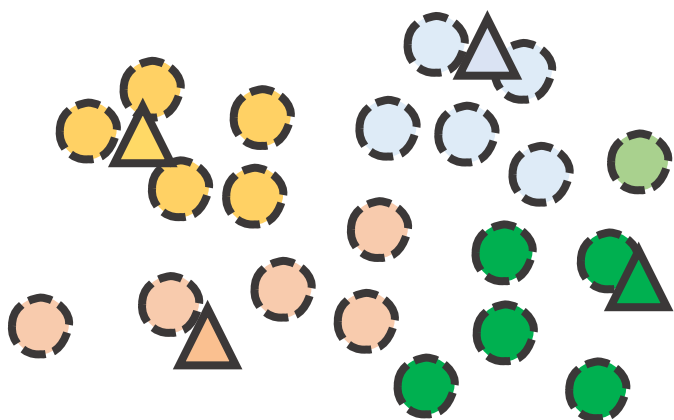


Random permutations do not
change the learned weights.
Exchangeability is maintained.

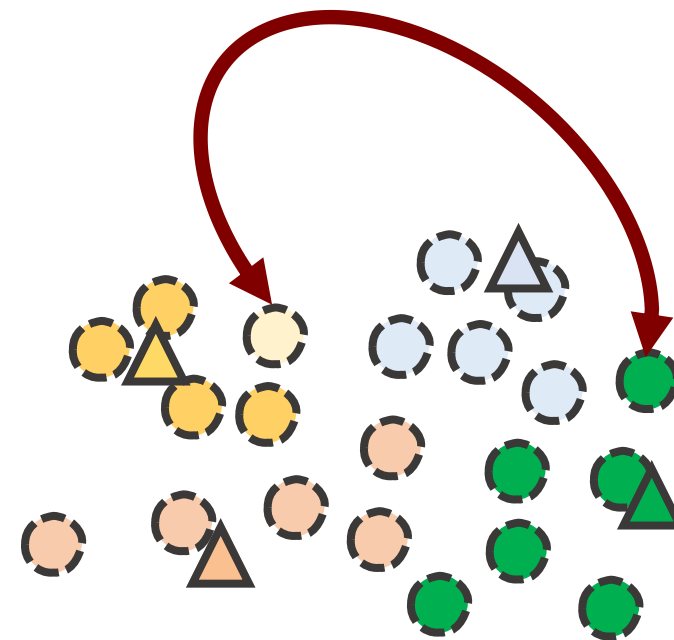


Our setting: full conformal adaptation

■ Interpretation



Exchange a train and
test point

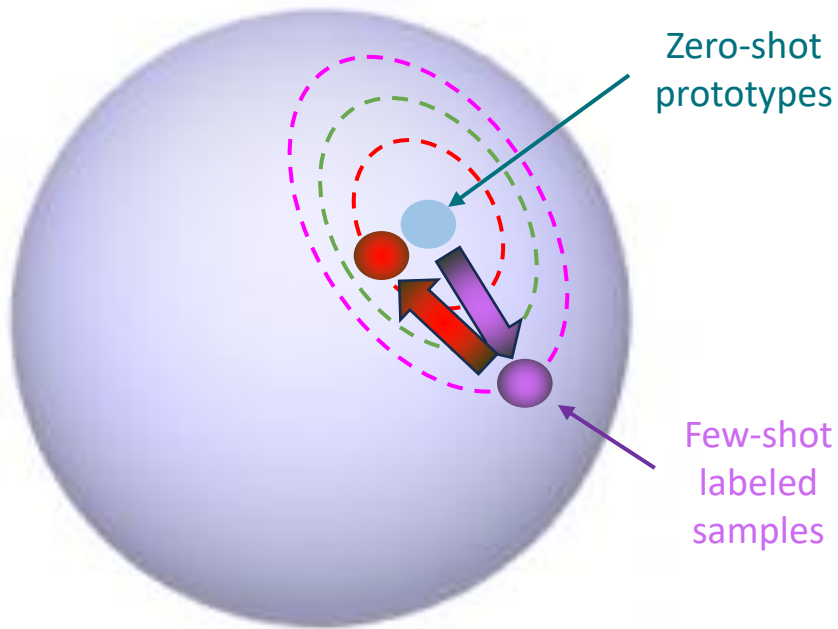


Random permutations do not
change the learned weights.
Exchangeability is maintained.

-  *Support sample (labeled)*
-  *Class prototype (learned)*
-  *Test point*

Training-free approximation for constrained linear probing

$$\min_{\mathbf{W}} \mathcal{L}(\mathbf{W}) = \underbrace{-\frac{1}{N} \sum_{i=1}^N \sum_{c=1}^C y_{ic} \ln(p_{ic}(\mathbf{W}))}_{\text{Cross-entropy on few-shots}} + \underbrace{\frac{\lambda}{2} \sum_{c=1}^C \|\mathbf{w}_c - \mathbf{t}_c\|_2^2}_{\text{Penalty if the solution deviates from the zero-shot prototypes}}$$



$$p_c(\mathbf{W}) = \frac{\exp(\mathbf{v}^\top \mathbf{w}_c / \tau)}{\sum_{j=1}^C \exp(\mathbf{v}^\top \mathbf{w}_j / \tau)}$$

Training-free approximation for constrained linear probing

$$\min_{\mathbf{W}} \mathcal{L}(\mathbf{W}) = -\frac{1}{N} \sum_{i=1}^N \sum_{c=1}^C y_{ic} \ln(p_{ic}(\mathbf{W})) + \frac{\lambda}{2} \sum_{c=1}^C \|\mathbf{w}_c - \mathbf{t}_c\|_2^2.$$

$$\mathcal{L} = g_1 + g_2$$

$$g_1 = -\frac{1}{N} \sum_{i=1}^N \sum_{c=1}^C y_{ic} (\mathbf{v}^\top \mathbf{w}_c / \tau) + \frac{\lambda}{2} \sum_{c=1}^C \|\mathbf{w}_c - \mathbf{t}_c\|_2^2$$

$$g_2 = \frac{1}{N} \sum_{i=1}^N \ln \left(\sum_{j=1}^C \exp(\mathbf{v}^\top \mathbf{w}_j / \tau) \right)$$

$$p_c(\mathbf{W}) = \frac{\exp(\mathbf{v}^\top \mathbf{w}_c / \tau)}{\sum_{j=1}^C \exp(\mathbf{v}^\top \mathbf{w}_j / \tau)}$$

Training-free approximation for constrained linear probing

$$\min_{\mathbf{W}} \mathcal{L}(\mathbf{W}) = -\frac{1}{N} \sum_{i=1}^N \sum_{c=1}^C y_{ic} \ln(p_{ic}(\mathbf{W})) + \frac{\lambda}{2} \sum_{c=1}^C \|\mathbf{w}_c - \mathbf{t}_c\|_2^2.$$

$$\mathcal{L} = g_1 + g_2$$

$$g_1 = -\frac{1}{N} \sum_{i=1}^N \sum_{c=1}^C y_{ic} (\mathbf{v}^\top \mathbf{w}_c / \tau) + \frac{\lambda}{2} \sum_{c=1}^C \|\mathbf{w}_c - \mathbf{t}_c\|_2^2$$

$$\frac{\partial g_1}{\partial \mathbf{w}_c} = -\frac{1}{N} \sum_{i=1}^N (y_{ic} \mathbf{v} / \tau) + \lambda (\mathbf{w}_c - \mathbf{t}_c)$$

$$\mathbf{w}_c^* = \arg \min_{\mathbf{w}_c} \frac{\partial g_1}{\partial \mathbf{w}_c} = \frac{1}{\lambda N \tau} \sum_{i=1}^N y_{ic} \mathbf{v} + \mathbf{t}_c$$

Visual prototypes

Textual

Training-free approximation for constrained linear probing

SS-Text solver:

$$\mathbf{w}_c^* = \frac{1}{\lambda N \tau} \sum_{i=1}^N y_{ic} \mathbf{v} + \mathbf{t}_c$$

Training-free approximation for constrained linear probing

SS-Text solver:

$$\mathbf{w}_c^* = \frac{1}{\lambda N \tau} \sum_{i=1}^N y_{ic} \mathbf{v} + \mathbf{t}_c$$

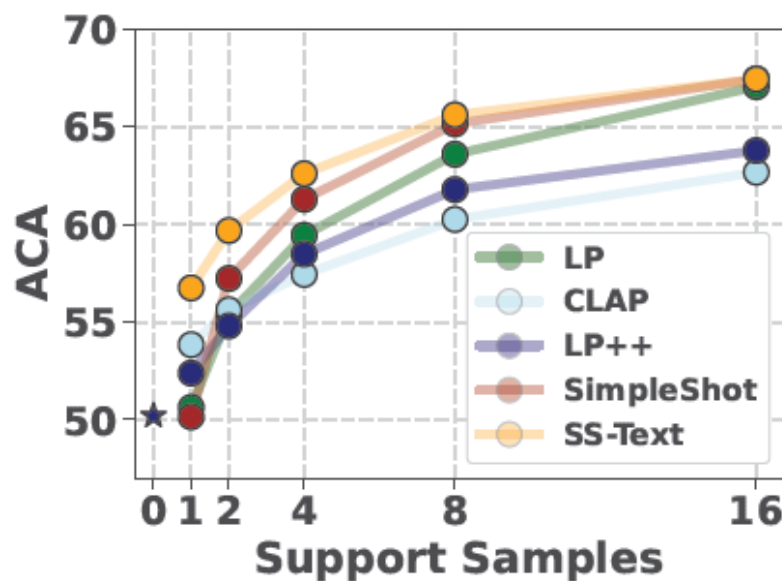

$$\lambda = 1/(N\tau)$$

$$\min_{\mathbf{W}} \mathcal{L}(\mathbf{W}) = -\frac{1}{N} \sum_{i=1}^N \sum_{c=1}^C y_{ic} \ln(p_{ic}(\mathbf{W})) + \frac{\lambda}{2} \sum_{c=1}^C \|\mathbf{w}_c - \mathbf{t}_c\|_2^2.$$

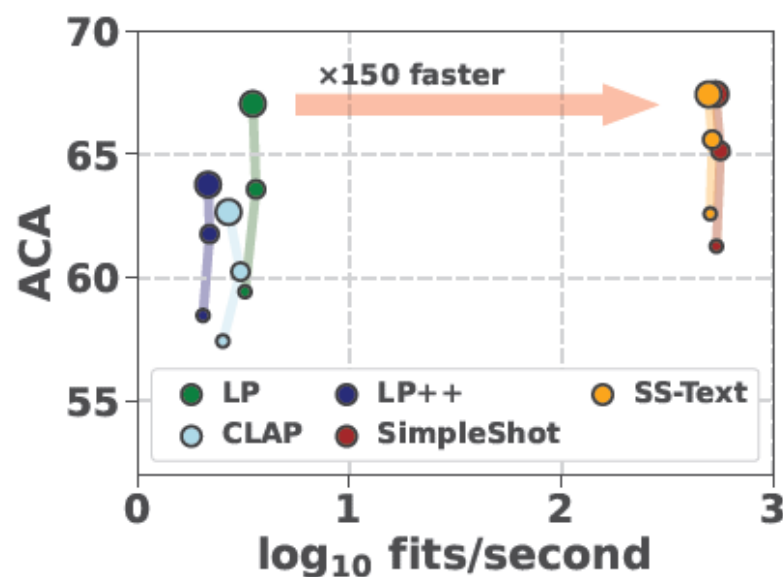
Training-free approximation for constrained linear probing

SS-Text solver:

$$\mathbf{w}_c^* = \frac{1}{\lambda N_\tau} \sum_{i=1}^N y_{ic} \mathbf{v} + \mathbf{t}_c$$



(a) Few-shot adaptation



(b) FCA Efficiency



Training-free approximation for constrained linear probing

SS-Text solver:

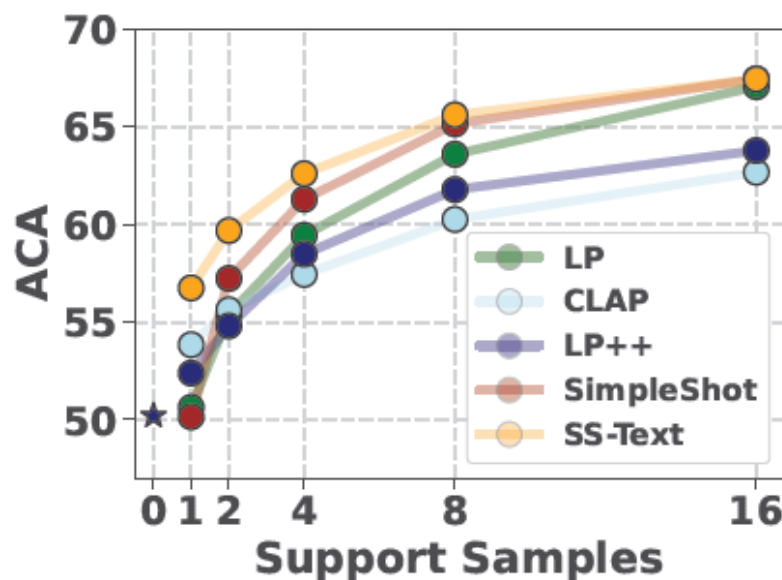
$$\mathbf{w}_c^* = \frac{1}{\lambda N \tau} \sum_{i=1}^N y_{ic} \mathbf{v} + \mathbf{t}_c$$

(in a particular use-case)

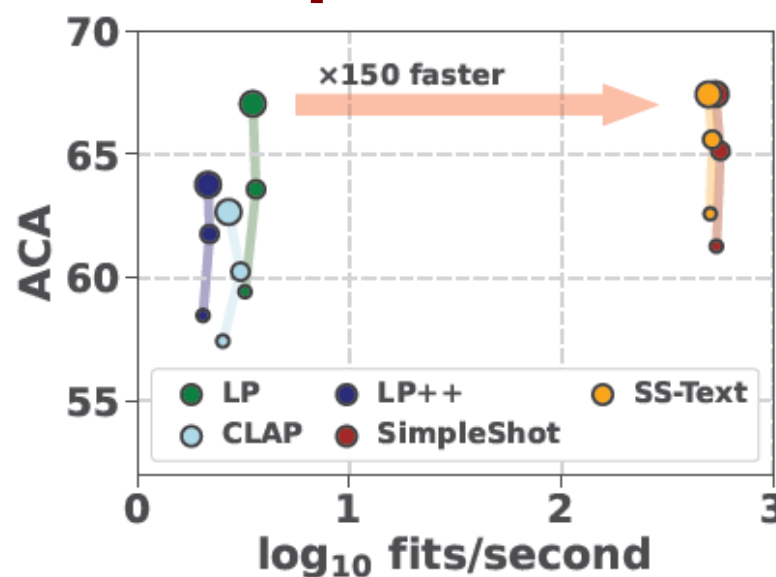
Skin (histology)

M=30.000, C=16

- LP: 23h
- SS-Text: 15min



(a) Few-shot adaptation



(b) FCA Efficiency

more shots

Conformal Prediction Results

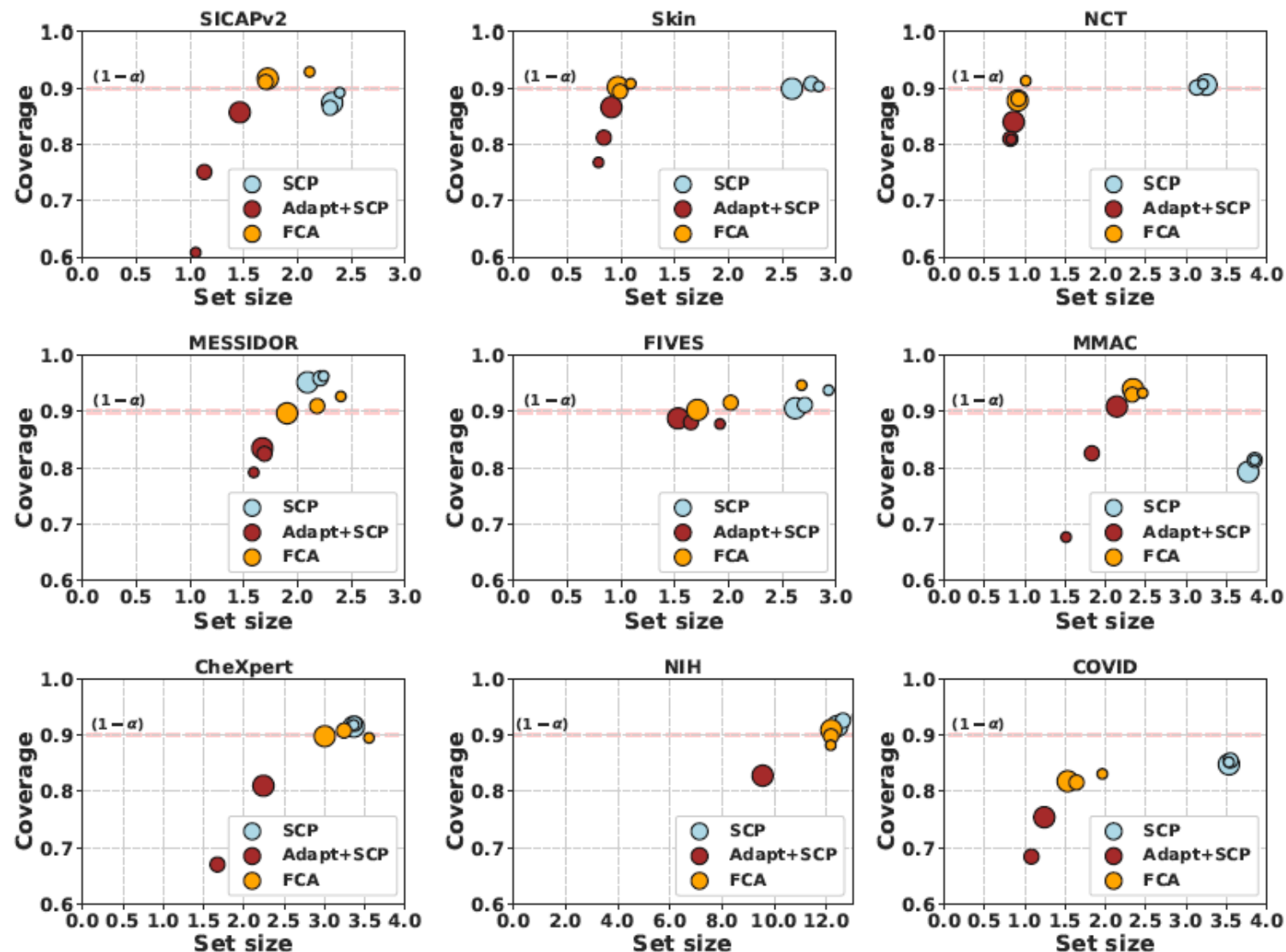
- Valid (finite-sample) coverage and strong discriminative performance

Method		$\alpha = 0.10$			
		ACA $\uparrow$	Cov.	Size $\downarrow$	CCV $\downarrow$
LAC	SCP	50.2	0.890	3.99	9.96
	Adapt+SCP	67.1 _{+16.9}	0.842	2.40 _{-1.59}	11.17 _{+1.21}
	FCA (<i>Ours</i>)	67.1 _{+16.9}	0.896	2.91 _{-1.08}	8.38 _{-1.58}
APS	SCP	50.2	0.900	4.05	9.59
	Adapt+SCP	67.1 _{+16.9}	0.858	2.56 _{-1.49}	8.57 _{-1.02}
	FCA (<i>Ours</i>)	67.1 _{+16.9}	0.898	3.06 _{-0.99}	6.12 _{-3.47}
RAPS	SCP	50.2	0.901	4.16	9.55
	Adapt+SCP	67.1 _{+16.9}	0.856	2.55 _{-1.61}	8.64 _{-0.91}
	FCA (<i>Ours</i>)	67.1 _{+16.9}	0.898	3.05 _{-1.11}	6.21 _{-3.34}

(16 labeled shots per class for adaptation)

Conformal Prediction Results

■ Per-dataset analysis



Conformal Prediction Results

- Qualitative assessment

Labeled	NC	1	2	3	4
	59.1	30.4	10.2	0.3	
	G3	27.0	57.9	14.3	0.8
	G4	21.1	66.2	11.8	0.9
	G5	76.8	19.3	3.4	0.5
		Set size			

(a) SICAPv2

Labeled	NC	G3	G4	G5
	94.1	48.5	16.2	1.1
	G3	28.8	92.6	69.5
	G4	10.9	77.3	89.1
	G5	2.8	7.1	27.7
		Categories in sets		

Labeled	N	1	2	3	4	5
	43.9	45.2	9.9	0.8	0.2	
	Pro. Sev. Mod. Mild.	18.8	61.5	18.2	0.6	0.9
	7.0	49.4	35.9	6.1	1.6	
	16.7	67.3	15.3	0.7	0.0	
		Set size				

(b) MESSIDOR

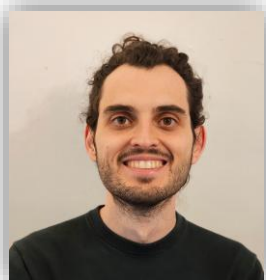
Labeled	N	Mild.	Mod.	Sev.	Prol.
	85.4	57.4	21.2	1.5	2.7
	Pro. Sev. Mod. Mild.	46.6	85.8	61.5	8.2
	19.5	62.0	90.4	60.8	14.0
	3.3	0.0	42.0	99.9	58.3
		Categories in sets			

Some take-home messages

- Medical **VLMs are strong black-box embedding models**. Its transfer potential allows us for data-efficient deployment scenarios.
- Conformal prediction is a promising ML framework for providing practitioners with **user-controlled, real-time guarantees**.
- **From focusing on “accuracy” to “efficiency”/“usefulness”**.
- Many aspects to explore yet, e.g., is **exchangeability** a realistic assumption in medical image analysis?

Full Conformal Adaptation of Medical Vision-Language Models

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Silva-Rodríguez



Leo
Fillioux



Paul-Henry
Cournède



Maria
Vakalopoulou



Stergios
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Ismail
Ben Ayed



Jose
Dolz



Few-shot adaptation results

- Ablation study on hyper-parameters for SS-text

Method	Setting	$K = 1$	$K = 2$	$K = 4$	$K = 8$	$K = 16$
Zero-shot [33]	(only text)	50.2	50.2	50.2	50.2	50.2
SimpleShot [47]	(only vision)	50.1	57.2	61.3	65.1	67.4
TIP-Adapter [51]	(training-free)	55.5	55.5	60.2	62.2	63.2
LP++ [14]	(training-free)	50.7	51.0	51.4	52.1	53.2
SS-Text	Fixed $\lambda = 0.1/\tau$	55.1	59.0	61.5	63.6	64.3
SS-Text	Fixed $\lambda = 1.0/\tau$	53.5	54.1	54.5	54.7	54.6
SS-Text	Fixed $\lambda = 10/\tau$	51.2	51.2	51.2	51.1	51.2
SS-Text	$\lambda_c \simeq$ zero-shot perf. [39]	51.4	58.4	62.6	65.7	67.4
SS-Text (<i>Ours</i>)	$\lambda = 1/(N\tau)$	56.7	59.7	62.6	65.6	67.4

Conformal Prediction Results

- More error rates

Method		$\alpha = 0.10$			$\alpha = 0.05$			
		ACA $\uparrow$	Cov.	Size $\downarrow$	CCV $\downarrow$	Cov.	Size $\downarrow$	CCV $\downarrow$
LAC	SCP	50.2	0.890	3.99	9.96	0.951	4.88	5.68
	Adapt+SCP	67.1_{+16.9}	0.842	2.40_{-1.59}	11.17 _{+1.21}	0.921	3.07_{-1.81}	6.87 _{+1.19}
	FCA (<i>Ours</i>)	67.1_{+16.9}	0.896	2.91 _{-1.08}	8.38_{-1.58}	0.952	3.56 _{-1.32}	5.02_{-0.66}
APS	SCP	50.2	0.900	4.05	9.59	0.952	4.88	5.54
	Adapt+SCP	67.1_{+16.9}	0.858	2.56_{-1.49}	8.57 _{-1.02}	0.924	3.19_{-1.69}	6.08 _{+0.54}
	FCA (<i>Ours</i>)	67.1_{+16.9}	0.898	3.06 _{-0.99}	6.12_{-3.47}	0.949	3.67 _{-1.21}	4.24_{-1.30}
RAPS	SCP	50.2	0.901	4.16	9.55	0.952	5.12	5.57
	Adapt+SCP	67.1_{+16.9}	0.856	2.55_{-1.61}	8.64 _{-0.91}	0.923	3.17_{-1.95}	6.12 _{+0.55}
	FCA (<i>Ours</i>)	67.1_{+16.9}	0.898	3.05 _{-1.11}	6.21_{-3.34}	0.951	3.66 _{-1.46}	4.23_{-1.34}

(16 labeled shots per class for adaptation)