



MAX PLANCK INSTITUTE  
FOR SOFTWARE SYSTEMS



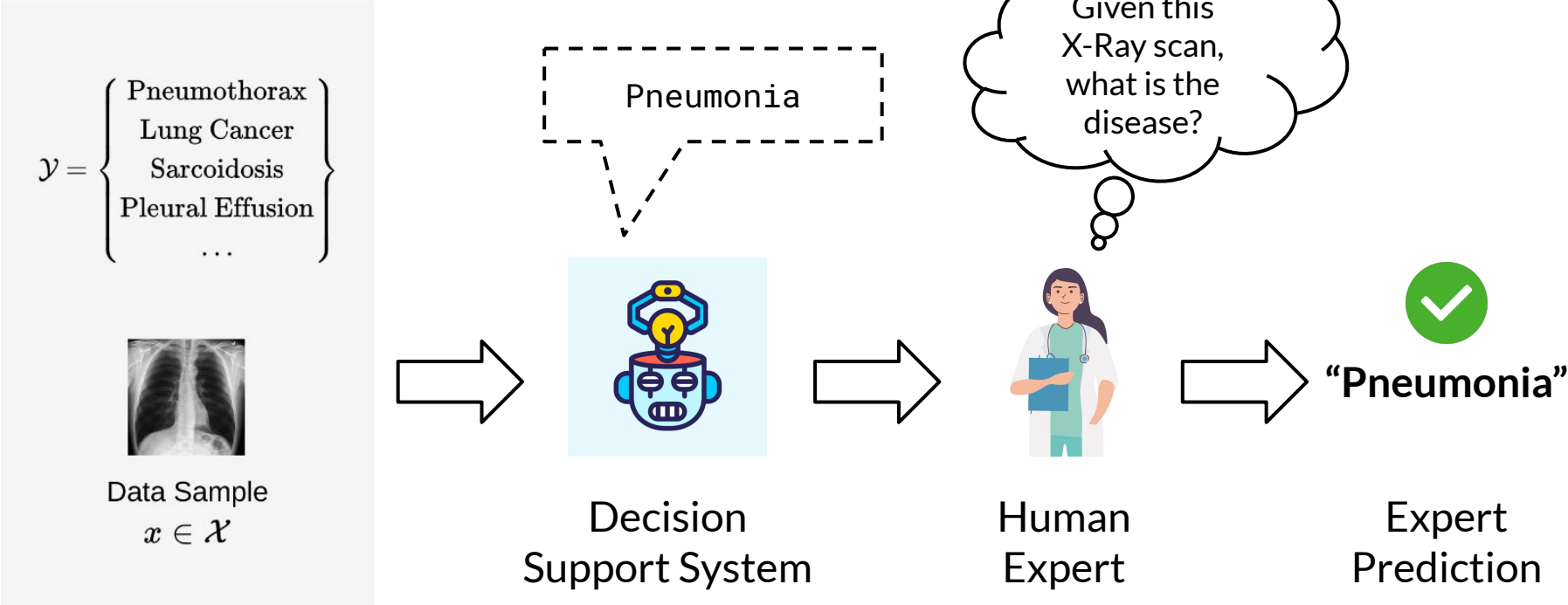
# Towards Human-AI Complementarity with Prediction Sets

**Giovanni De Toni<sup>1</sup>, Nastaran Okati<sup>2</sup>, Suhas Thejaswi<sup>2</sup>,  
Eleni Straitouri<sup>2</sup>, Manuel Gomez-Rodriguez<sup>2</sup>**

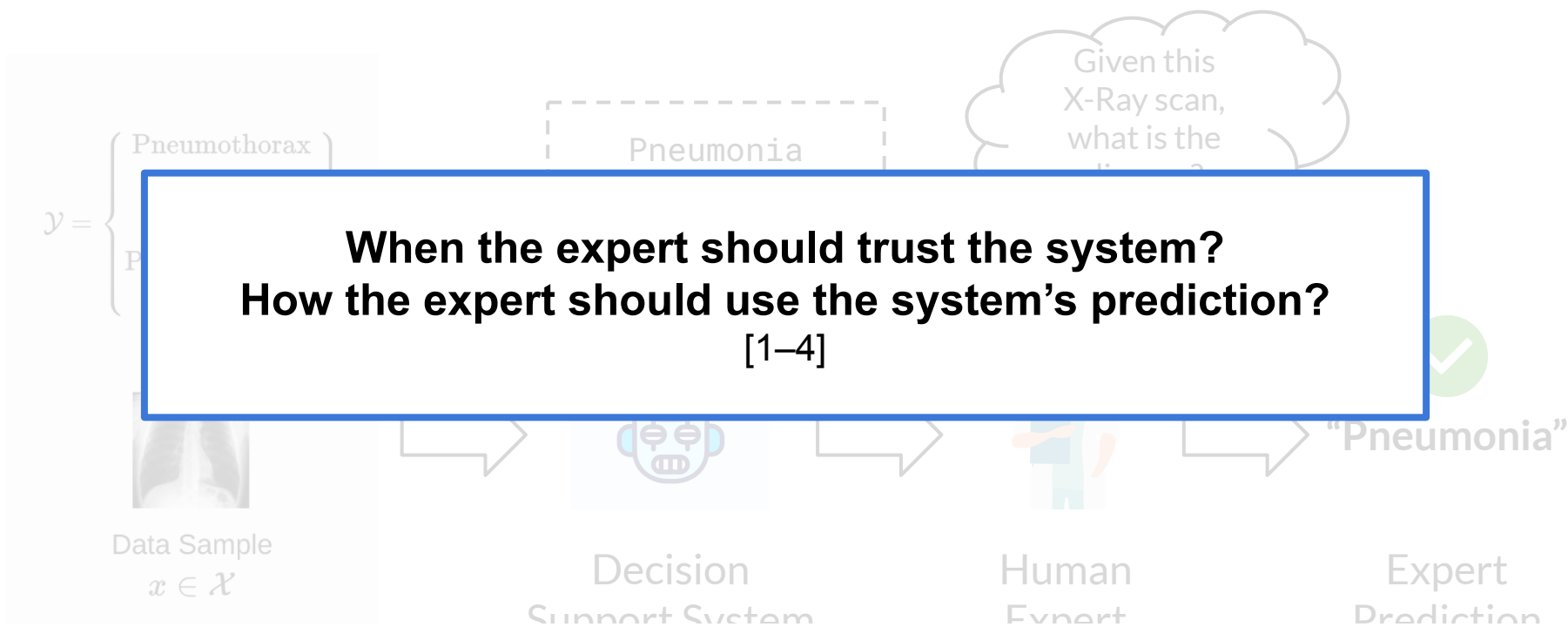
<sup>1</sup>Fondazione Bruno Kessler & University of Trento

<sup>2</sup>Max Planck Institute for Software Systems

# Decision Support System for multiclass classification



# Decision Support System for multiclass classification



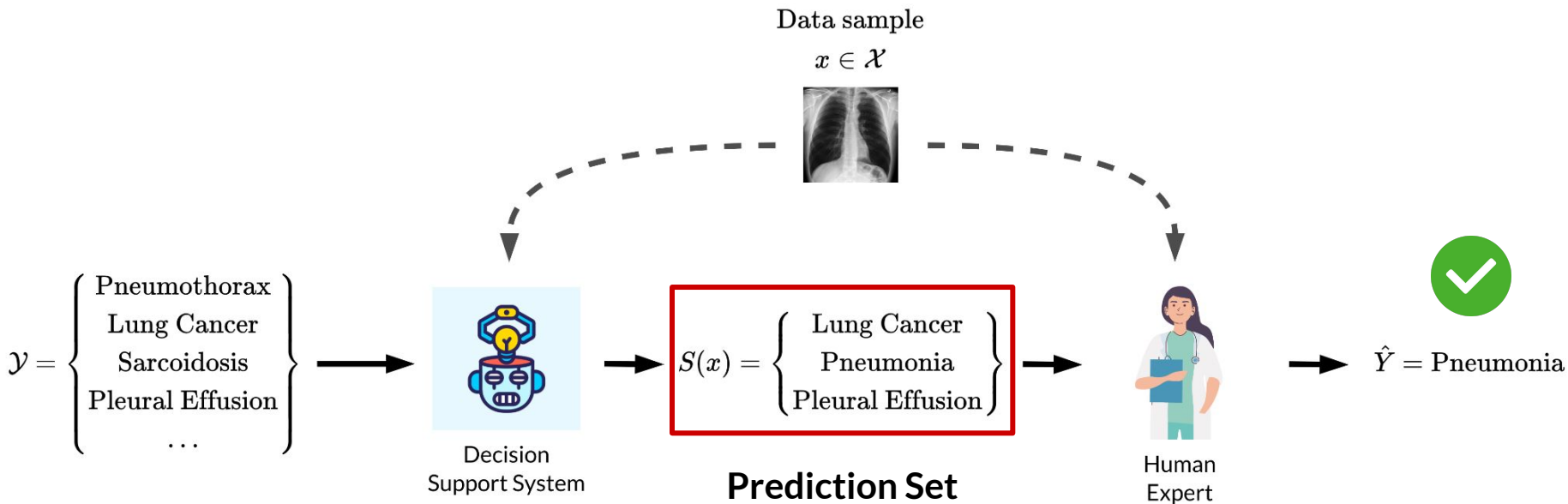
[1] Yin et al., Understanding the effect of accuracy on trust in machine learning models, CHI (2019)

[2] Zhang et al., Effect of confidence and explanation on accuracy and trust calibration in ai-assisted decision making, FAccT (2020)

[3] Suresh et al., Misplaced trust: Measuring the interference of machine learning in human decision-making, WebSci (2020)

[4] Lai et al., Towards a science of human-ai decision making: a survey of empirical studies, Preprint (2021)

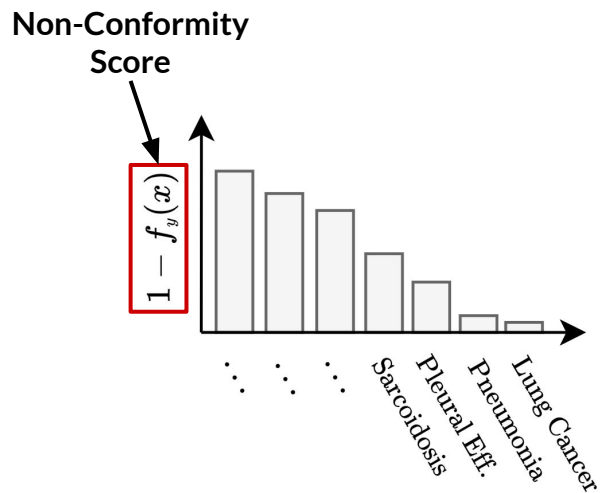
# Alternative Support Systems based on prediction sets [5,6]



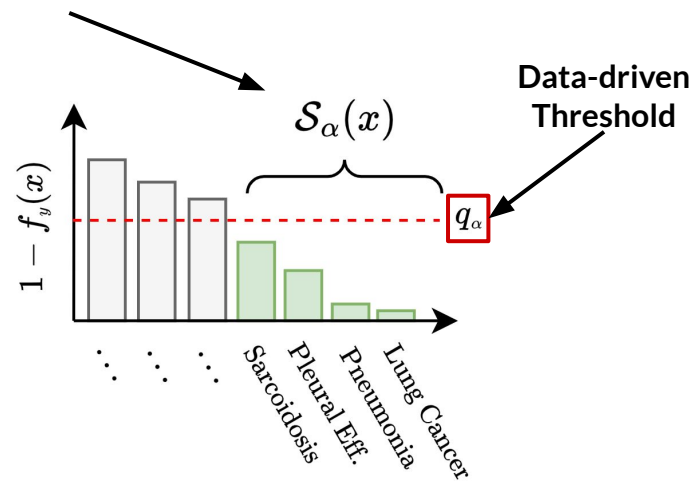
[5] Straitouri et al., Improving expert predictions with conformal prediction, ICML (2023)

[6] Eleni Straitouri and Manuel Gomez-Rodriguez, Designing decision support systems using counterfactual prediction sets, ICML (2024)

# Prediction sets with Conformal Prediction [7,8]



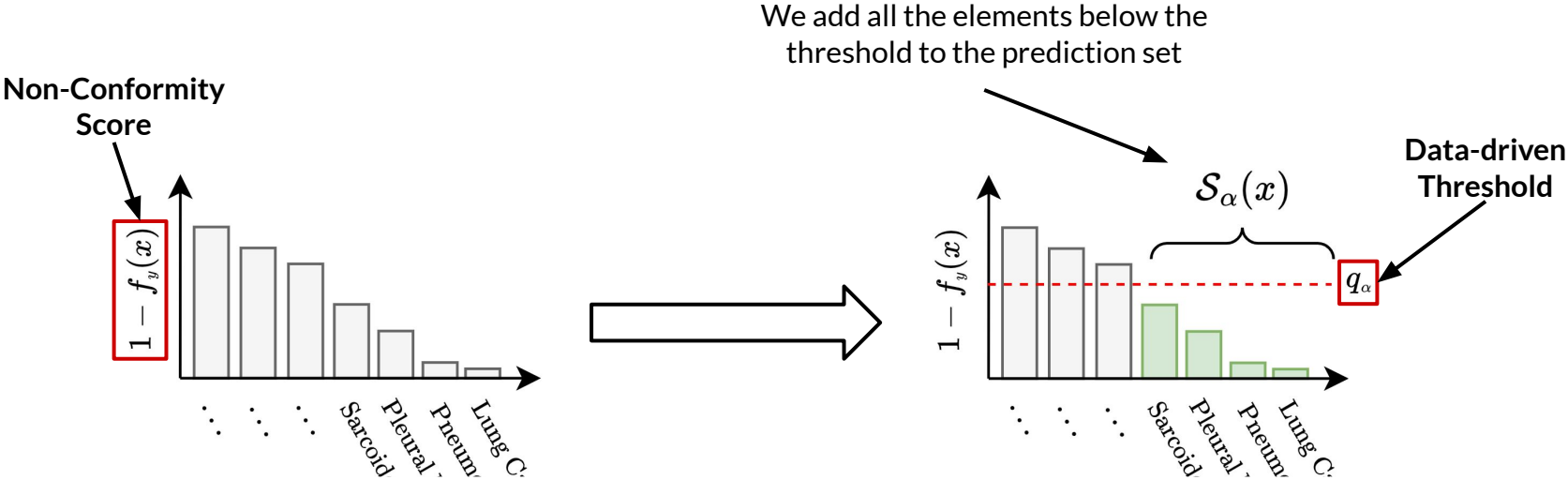
We add all the elements below the threshold to the prediction set



[7] Vladimir Vovk, Alexander Gammerman, and Glenn Shafer, Algorithmic learning in a random world, Vol. 29. New York: Springer (2005)

[8] Anastasios N. Angelopoulos, and Stephen Bates, Conformal prediction: A gentle introduction, Foundations and Trends® in Machine Learning (2023)

# Prediction sets with Conformal Prediction [7,8]



Coverage guarantees:

$$P(y \in \mathcal{S}_\alpha(\text{Instance})) \geq 1 - \alpha$$

True Label

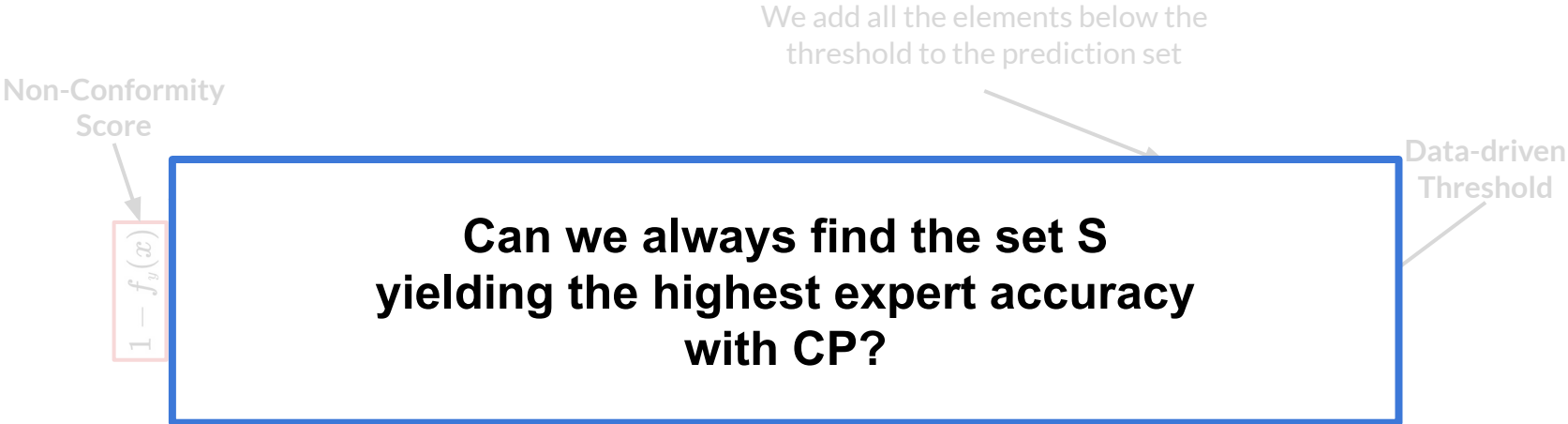
Prediction Set

Instance

Target Probability

[7] Vladimir Vovk, Alexander Gammerman, and Glenn Shafer, Algorithmic learning in a random world, Vol. 29. New York: Springer (2005)  
 [8] Anastasios N. Angelopoulos, and Stephen Bates, Conformal prediction: A gentle introduction, Foundations and Trends® in Machine Learning (2023)

# Prediction sets with Conformal Prediction [7,8]



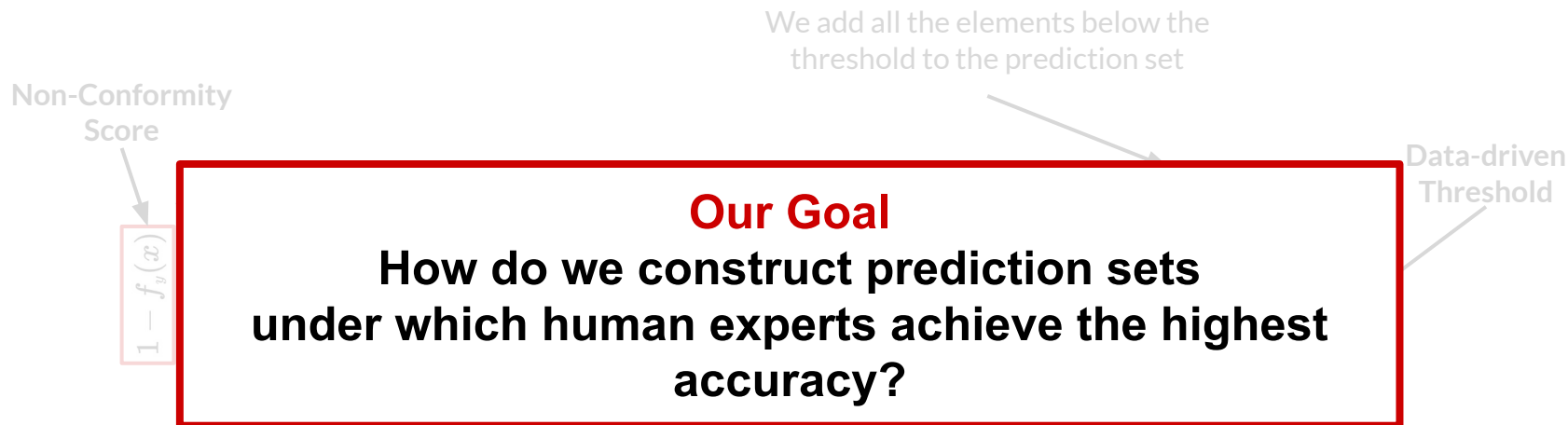
Coverage guarantees:

$$P(y \in \mathcal{S}_\alpha(\text{Instance})) \geq 1 - \alpha$$

True Label      Prediction Set      Instance      Target Probability

[7] Vladimir Vovk, Alexander Gammerman, and Glenn Shafer, Algorithmic learning in a random world, Vol. 29. New York: Springer (2005)  
[8] Anastasios N. Angelopoulos, and Stephen Bates, Conformal prediction: A gentle introduction, Foundations and Trends® in Machine Learning (2023)

# Prediction sets with Conformal Prediction [7,8]



Coverage guarantees:

$$P(y \in \mathcal{S}_\alpha(\text{Instance})) \geq 1 - \alpha$$

True Label      Prediction Set      Instance      Target Probability

[7] Vladimir Vovk, Alexander Gammerman, and Glenn Shafer, Algorithmic learning in a random world, Vol. 29. New York: Springer (2005)

[8] Anastasios N. Angelopoulos, and Stephen Bates, Conformal prediction: A gentle introduction, Foundations and Trends® in Machine Learning (2023)



# How can we build sets maximizing the expert's accuracy?

We approximate the expert as a multinomial logit model (MNL) [5,9]

Probability the expert picks  $y$  from  $\mathcal{S}$  when  $y$  is the true label

$$g(\mathcal{S} \mid x) = \sum_{y \in \mathcal{S}} f_y(x) \frac{C_{yy}}{\sum_{y' \in \mathcal{S}} C_{y'y}}$$

**Estimator of the expert's accuracy**

# How can we build sets maximizing the expert's accuracy?

We approximate the expert as a multinomial logit model (MNL) [5,9]

Probability the expert picks  $y$  from  $\mathcal{S}$  when  $y$  is the true label

$$g(\mathcal{S} | x) = \sum_{y \in \mathcal{S}} f_y(x) \frac{C_{yy}}{\sum_{y' \in \mathcal{S}} C_{y'y}}$$

Estimator of the expert's accuracy

**Goal**

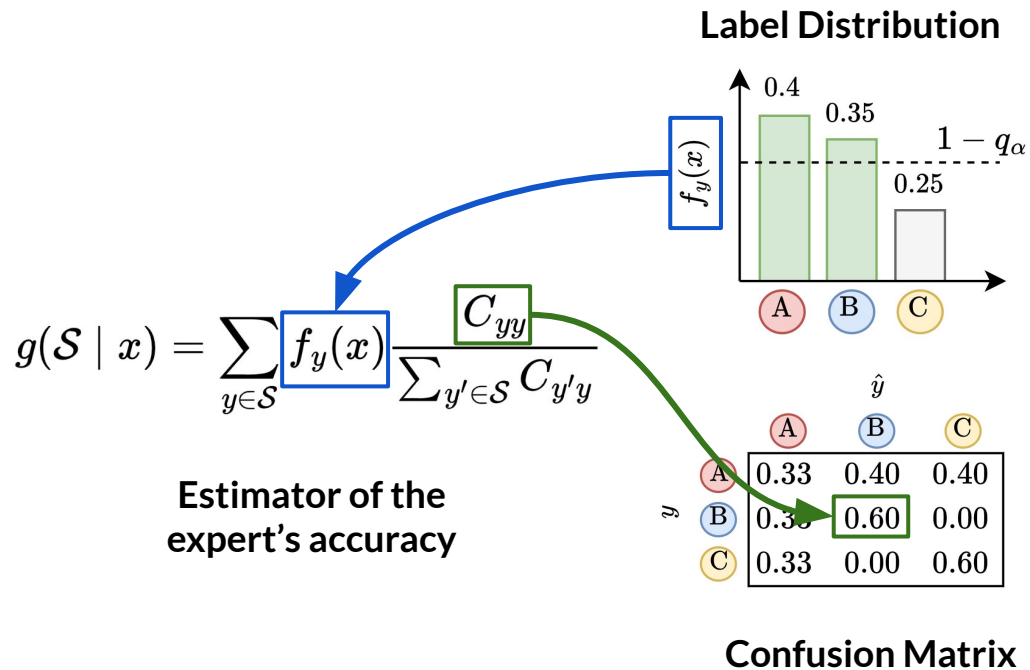
Find the prediction set maximizing the expert accuracy:

$$\mathcal{S}^* = \operatorname{argmax}_{\mathcal{S} \subseteq \mathcal{Y}} g(\mathcal{S} | x)$$

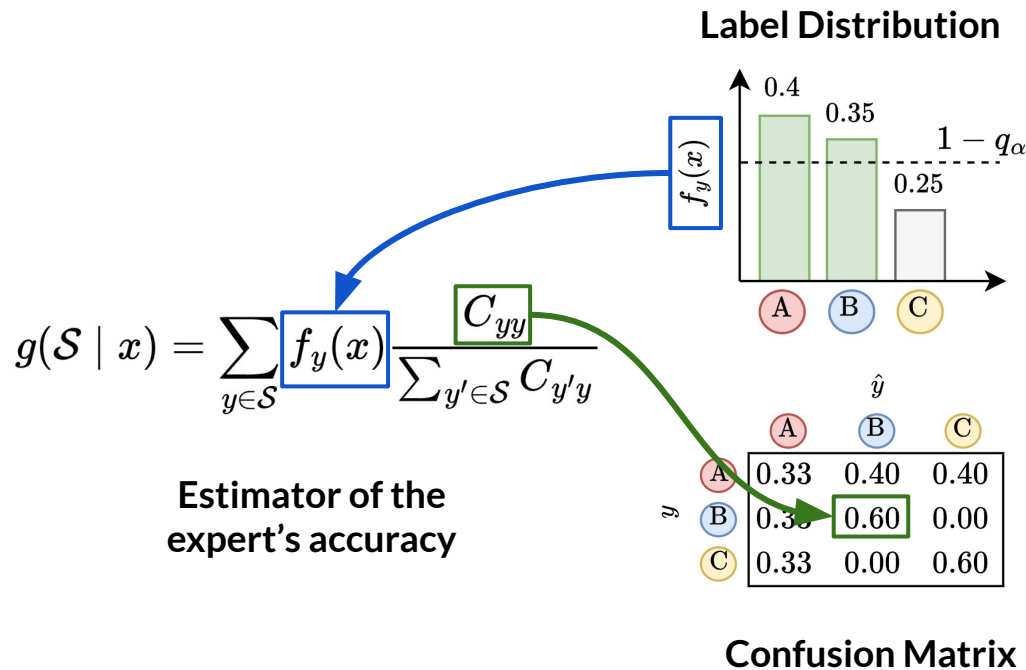
where:

$$g(\mathcal{S} | x) = \sum_{y \in \mathcal{S}} f_y(x) \frac{C_{yy}}{\sum_{y' \in \mathcal{S}} C_{y'y}}$$

# Conformal Prediction is **suboptimal**



# Conformal Prediction is **suboptimal**



All possible (conformal) prediction sets

$$g(\mathcal{S}_{cp} | x) = \begin{cases} 0.49 & \mathcal{S}_{cp} = \{A, B, C\} \\ 0.41 & \mathcal{S}_{cp} = \{A, B\} \\ 0.4 & \mathcal{S}_{cp} = \{A\} \end{cases}$$

!  $g(\{B, C\} | x) = 0.60$

There is a set with a higher objective!

# Finding the optimal prediction set is hard

## Goal

Find the prediction set maximizing the expert accuracy:

$$\mathcal{S}^* = \operatorname{argmax}_{\mathcal{S} \subseteq \mathcal{Y}} g(\mathcal{S} \mid x)$$

where:

$$g(\mathcal{S} \mid x) = \sum_{y \in \mathcal{S}} f_y(x) \frac{C_{yy}}{\sum_{y' \in \mathcal{S}} C_{y'y}}$$

Finding the optimal set is **NP-Hard** and it is **NP-hard to approximate** to any non-trivial factor\*

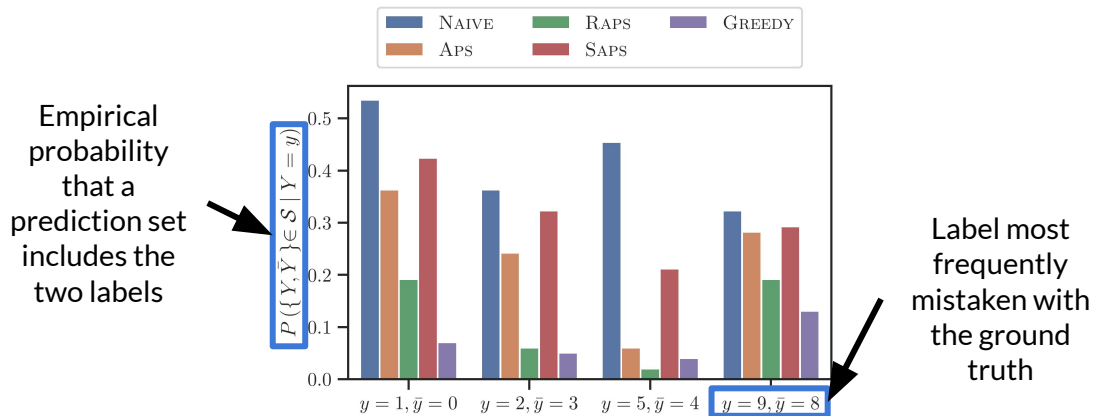
\* Our reduction is from the  $k$ -clique and maximum clique problems, respectively.

**Greedy algorithm guaranteed to offer equal or greater performance than CP**

# Our greedy algorithm

Highest accuracy than CP in simulation studies with both **synthetic** and **real expert predictions**

Less likely to include labels the expert would **mistake** for the true label



Come to our poster on  
Wednesday 11th  
11 a.m. – 2 p.m. PST

