Active Learning - the pool-based selective sampling (part 1)

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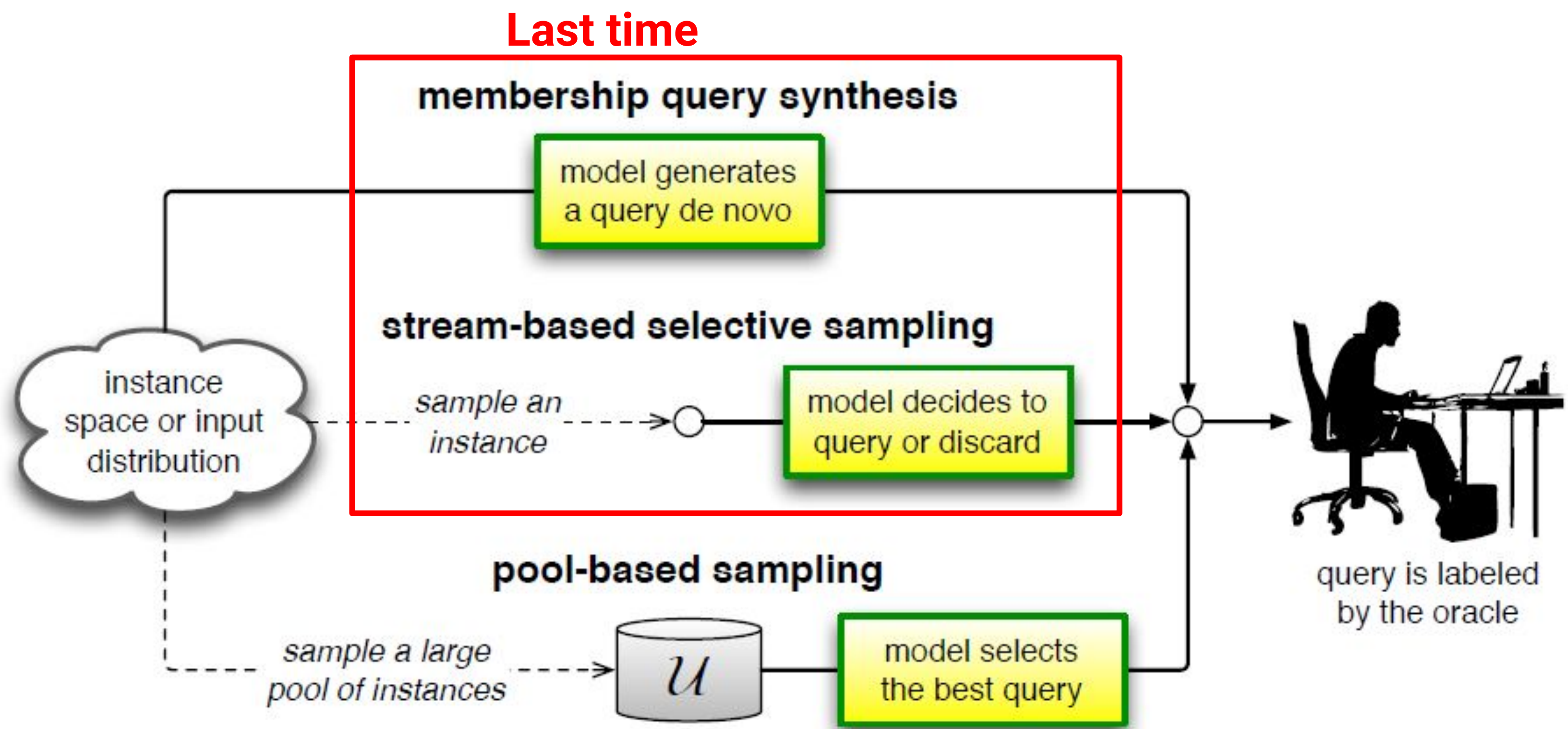
THE PLAN

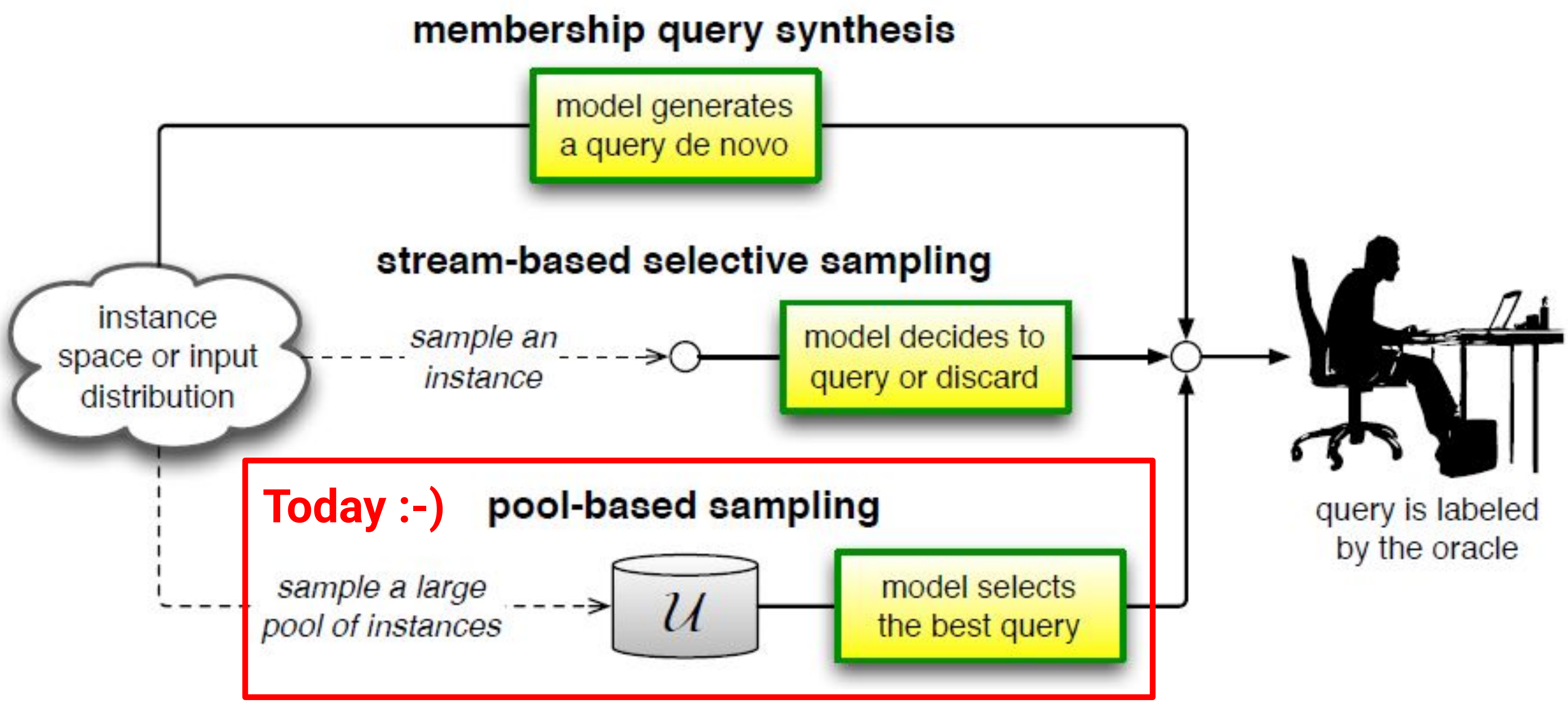
- A recap of the previous lecture.
- Uncertainty sampling.
- Exemplary measures.
- Use-cases.
- Evaluation in active learning experiments.
- Summary.

The three main Active Learning scenarios



Based on *Burr Settles: Active Learning Literature Survey (2010)*

The three main Active Learning scenarios



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Active Learning as an optimization task

Formal task definition - we search for $U^* \subset DP$ such that:

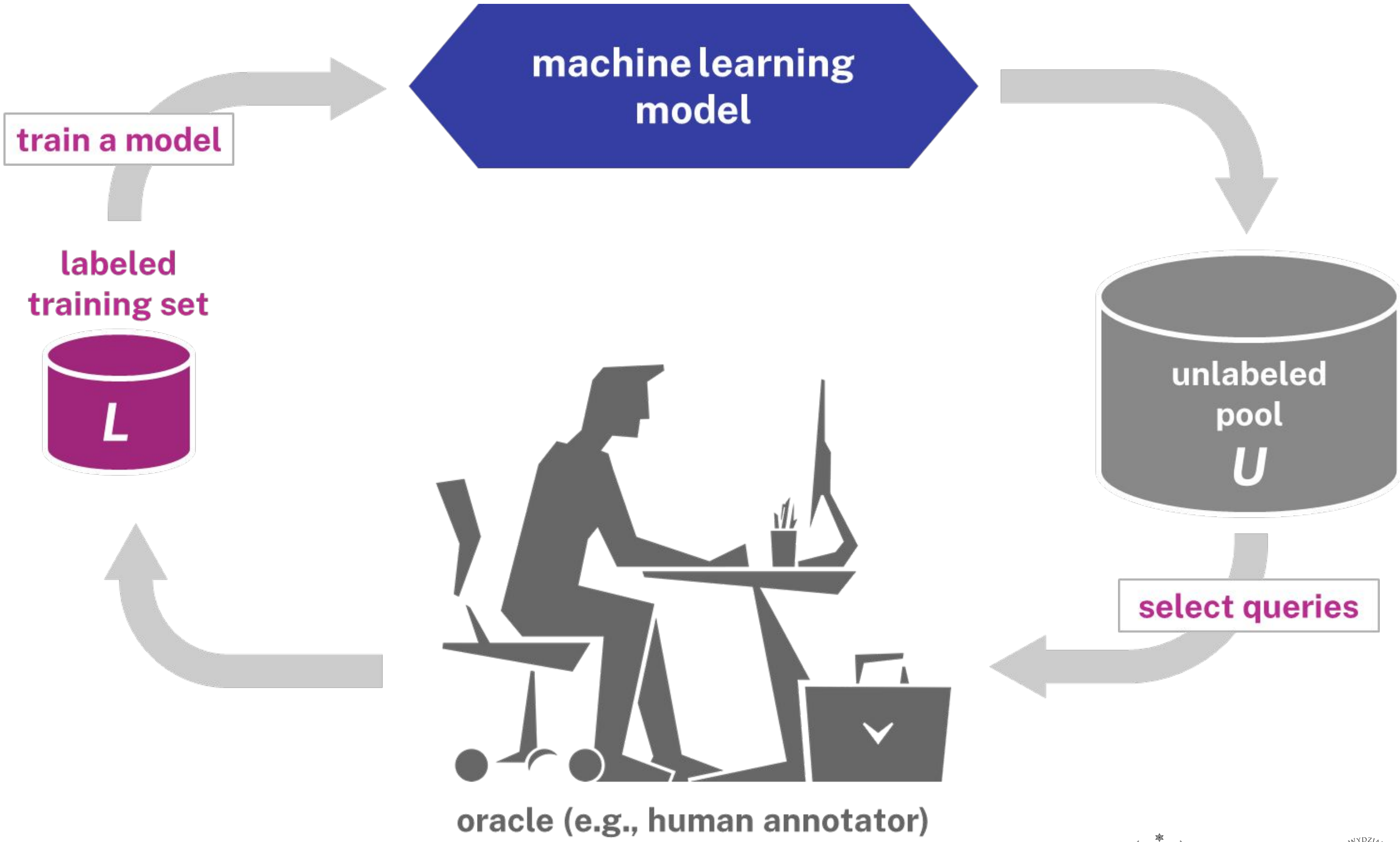
$$U^* = \underset{U:|U|=K}{\arg\max}\ \mathbb{E}_{(X,Y)}[q(Y, f^U(X))]$$

where f^U is a model trained on a subset $U \subset DP$ whose size is *K* and *q* is a predefined quality metric.

Pool-based selective sampling

- We have a large pool of unlabeled instances *U*.
  - We evaluate the usefulness of the instances from *U* for the learner <u>at each iteration of the AL cycle</u>.
  - We may choose one or more instances to query the oracle.
  - The unlabeled data pool may grow in time but we assume that it is static in each iteration.
- An informativeness measure is used to evaluate all instances from the pool.
  - If the pool size is very large, some subsampling can be used…
- **How do we evaluate the informativeness of an instance?**

The active learning cycle - revisited



An example - Cancer tissue classification

- Rączkowski et al. (2019) describe an application of the pool-based active learning in the field of medical diagnostics.
  - Active learning framework chooses uncertain samples.
  - Instances - small tiles with tissues stained with hematoxylin and eosin (H&E).
  - Histopathologists annotate pixels of the image with tissue classes.
  - Deep neural network is used to learn from the annotated examples.
- The active learning approach resulted in 45% speed-up of the model learning process.

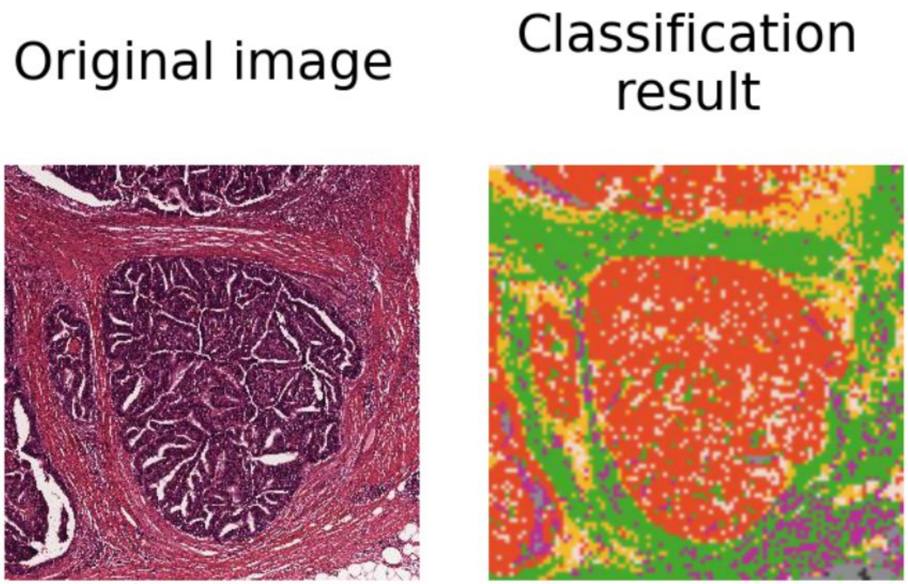
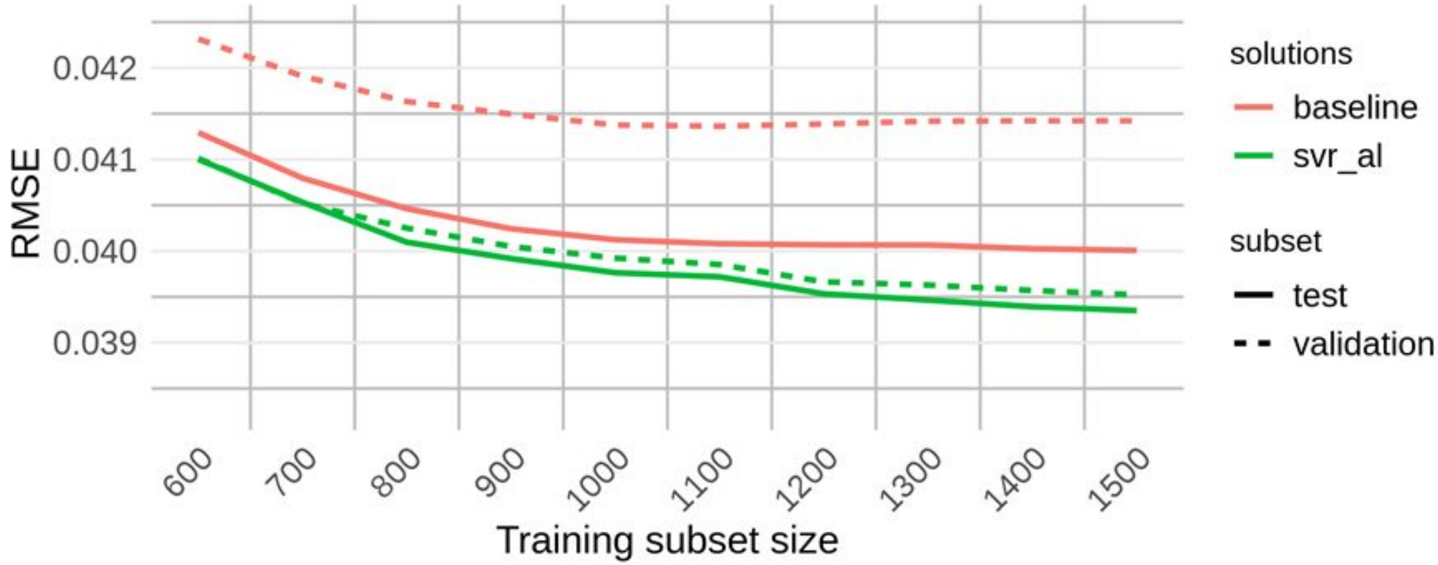


Image taken from Rączkowski et al. (2019): ARA: accurate, reliable and active histopathological image classification framework with Bayesian deep learning.

Image: Freepik.com

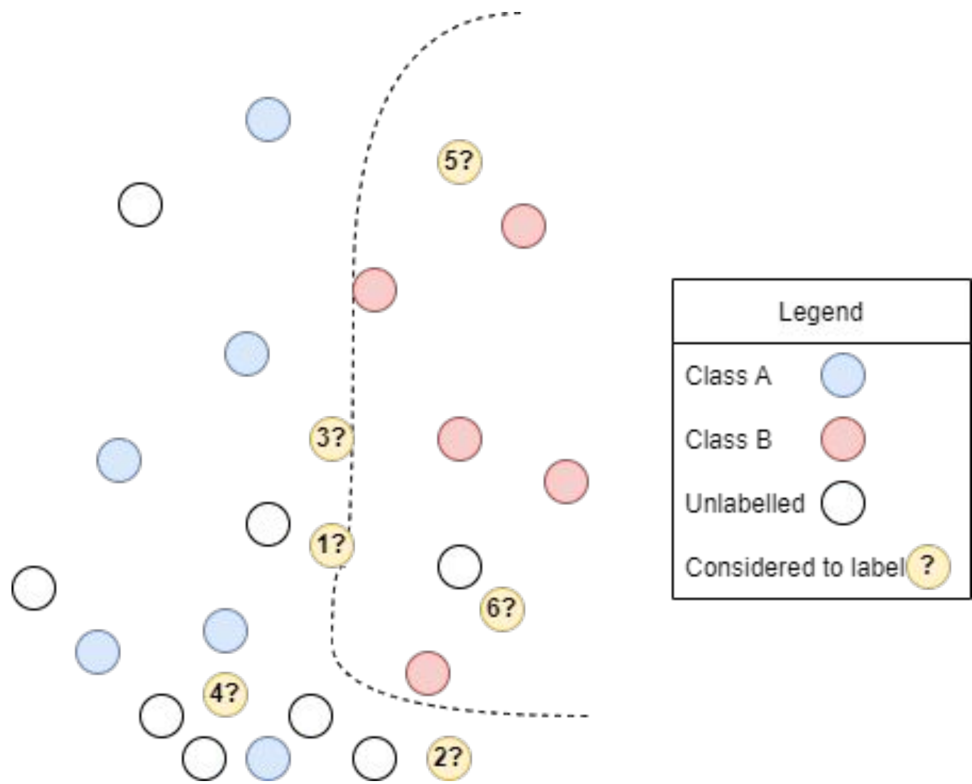
An exemplary application - AAIA’19 DMC



- Janusz et al. (2019) proposed a method based on a combination of informativeness density and diversity sampling for active learning of deck win-rates in a popular mobile video game Clash Royale.
- Historical win-rates were available for a large pool of decks. How will the win-rates change in a new season?
- Active learning outperformed random sampling and nu-SVR baselines. https://knowledgepit.ml/clash-royale-challenge/

Informativeness and uncertainty - again

- The informativeness can be considered from several perspectives:
  - Proximity to a decision boundary ≈ prediction uncertainty.
  - Representativeness.
  - Expected impact on the learner.
  - Expected influence on the lerner's generalization quality.



Uncertainty sampling

- The simplest and very popular approach:
  - We evaluate the prediction uncertainty for each instance.
    - For the classification task, it boils down to querying near the decision boundary region.
  - We want to minimize the epistemic uncertainty of the learner.
  - Measuring the epistemic uncertainty is not easy…
- All we need is a good measure.
  - How can we measure the proximity to the decision boundary?
  - What about the regression task?
  - What changes for the multi-label classification?
  - Other ML tasks?

Classification uncertainty sampling

- Popular classification uncertainty sampling methods:
  - Least confidence: $u^*_{LC} = \arg\max_u (1 - P_\theta(\hat{y}|u))$
  - Minimum margin: $u^*_M = \arg\min_u (P_\theta(\hat{y}_1|u) - P_\theta(\hat{y}_2|u))$
  - Shannon entropy: $u^*_H = \arg\max_u \left(-\sum_i P_\theta(y_i|u) \log P_\theta(y_i|u) \right)$
- Many other measures are vailable…
- **But most of the commonly used measures assume uniformly distributed decision thresholds!**

Classification uncertainty - analysis

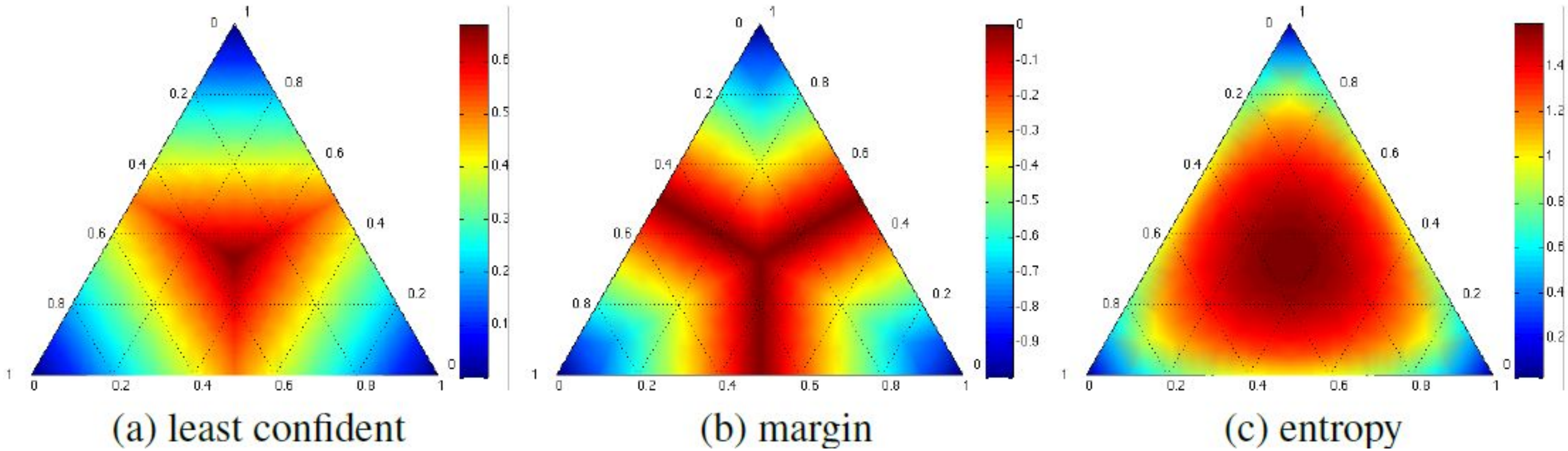
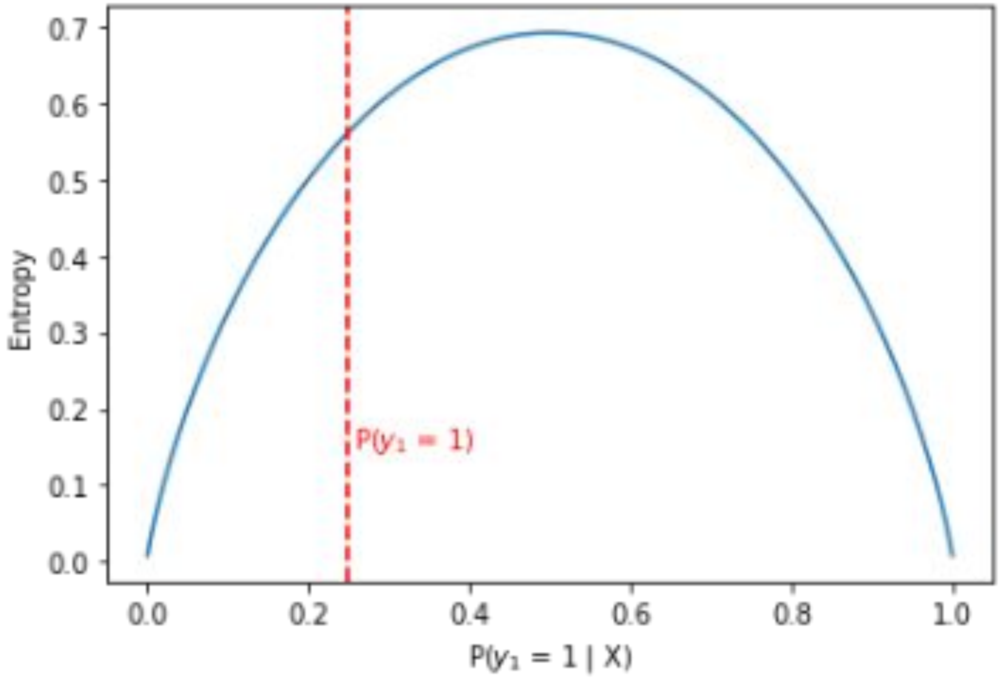


Image taken from Burr Settles: Active Learning Literature Survey (2010)

Imbalanced classification problems

- What if the class distribution is imbalanced and the quality measure gives different weights to classes?
  - We may want to shift the decision thresholds!



Informativeness for imbalanced classification

- Standard uncertainty measures can be adjusted so that they take their maximum at any given class distribution.
  - A simple rescaling trick!

$$< p_1, \ldots, p_i, \ldots, p_k > \ \text{-} \ \textit{predicted distribution}$$

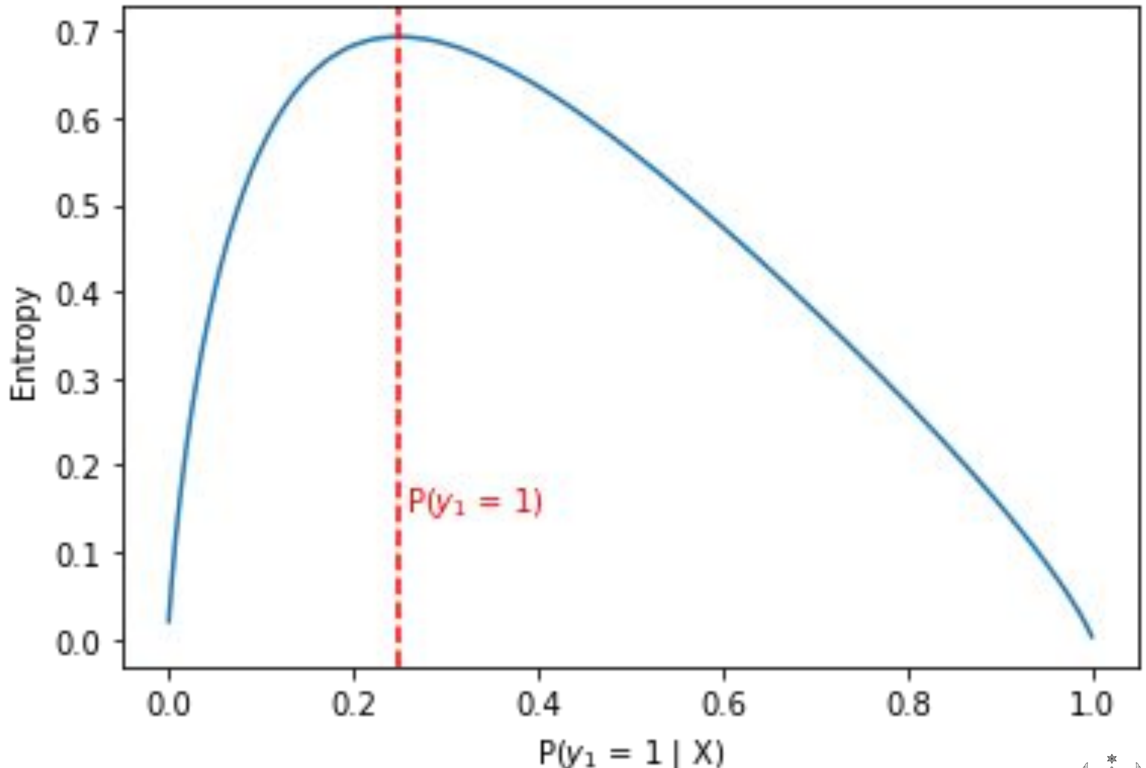
$$< r_1, \ldots, r_i, \ldots, r_k > \ \text{-} \ \textit{target distribution}$$

$$Let\ c = \sum_{i=1,\ldots,k} \frac{p_i}{r_i},\ then\ p_i \longrightarrow \frac{1}{c} \cdot \frac{p_i}{r_i}$$

- **How to choose the right decision boundary?**

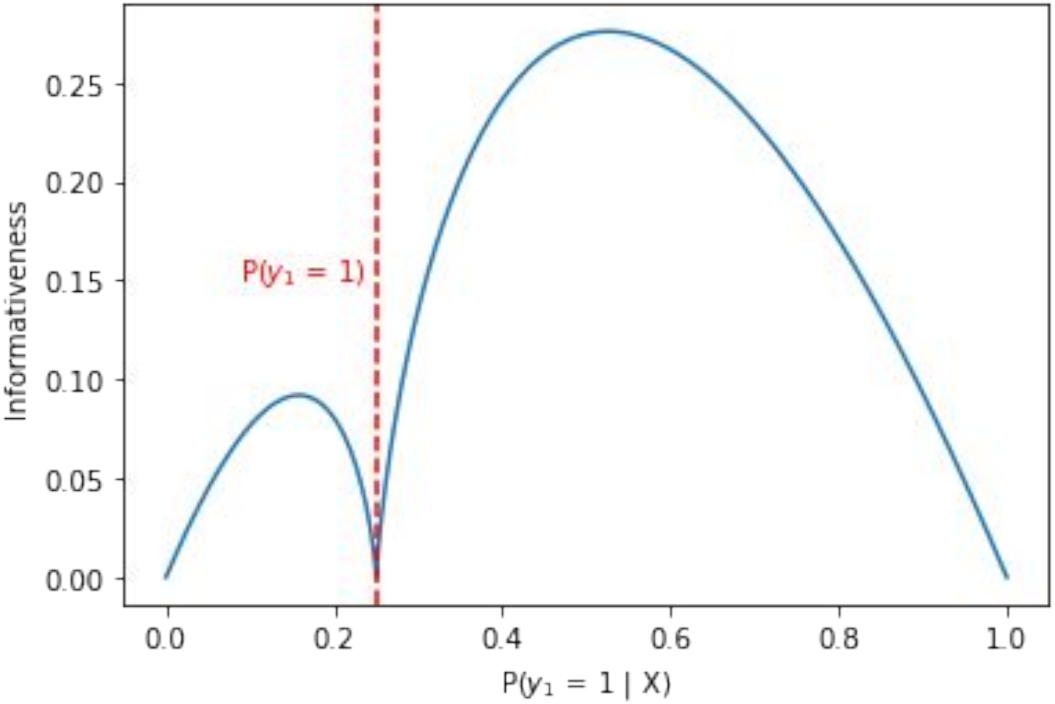
Rescaled decision boundaries

- If we consider a decision threshold at 0.25, we get a “decision threshold-centered entropy” :-)

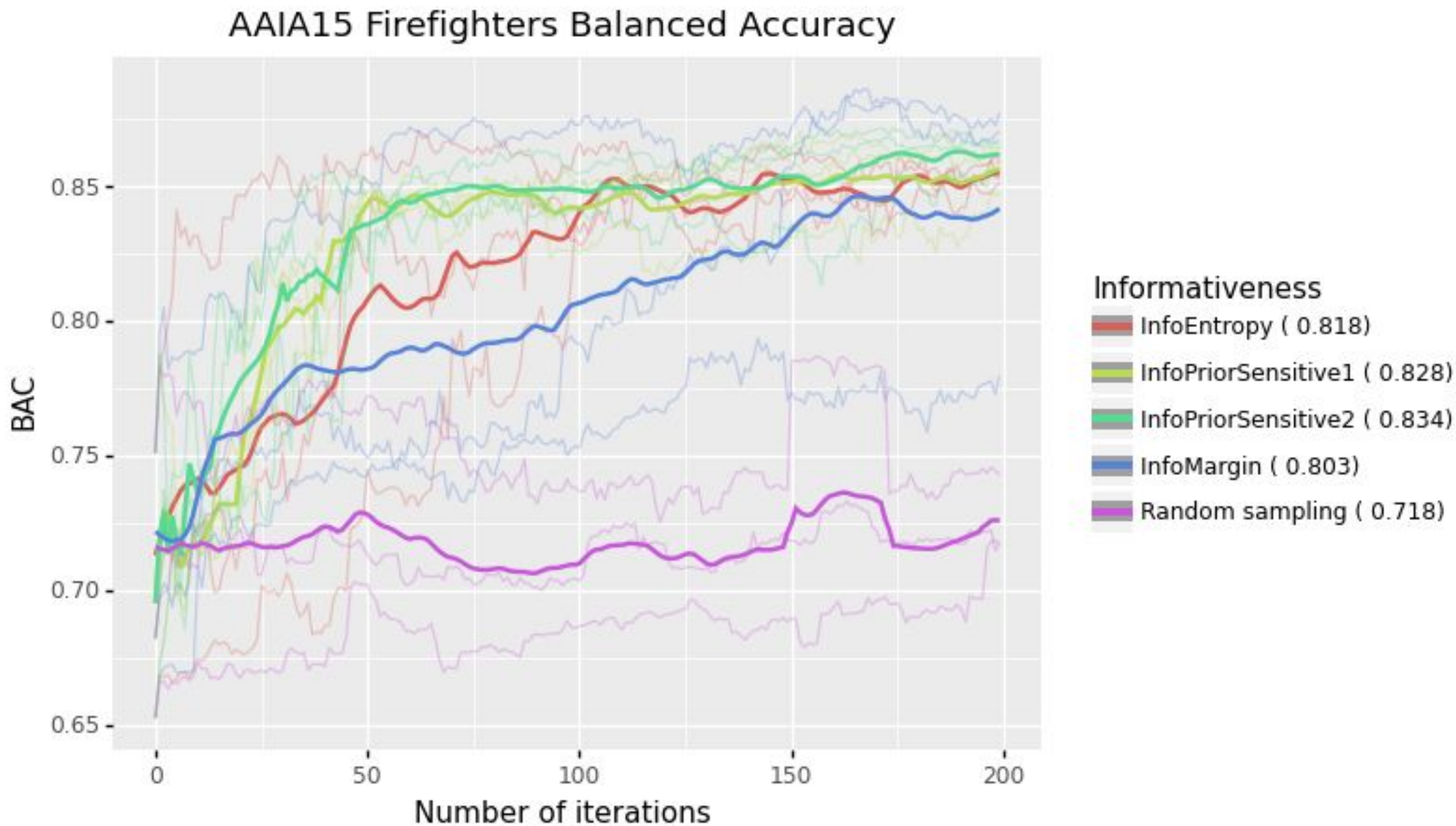


Other ideas

- What if we don't want to promote sampling from the decision boundary?
  - Cases very near to the boundary can be confusing to experts (i.e., our oracle).
  - Cases might be close to the boundary due to aleatoric uncertainty.



An example - a comparison on AAIA’15 data

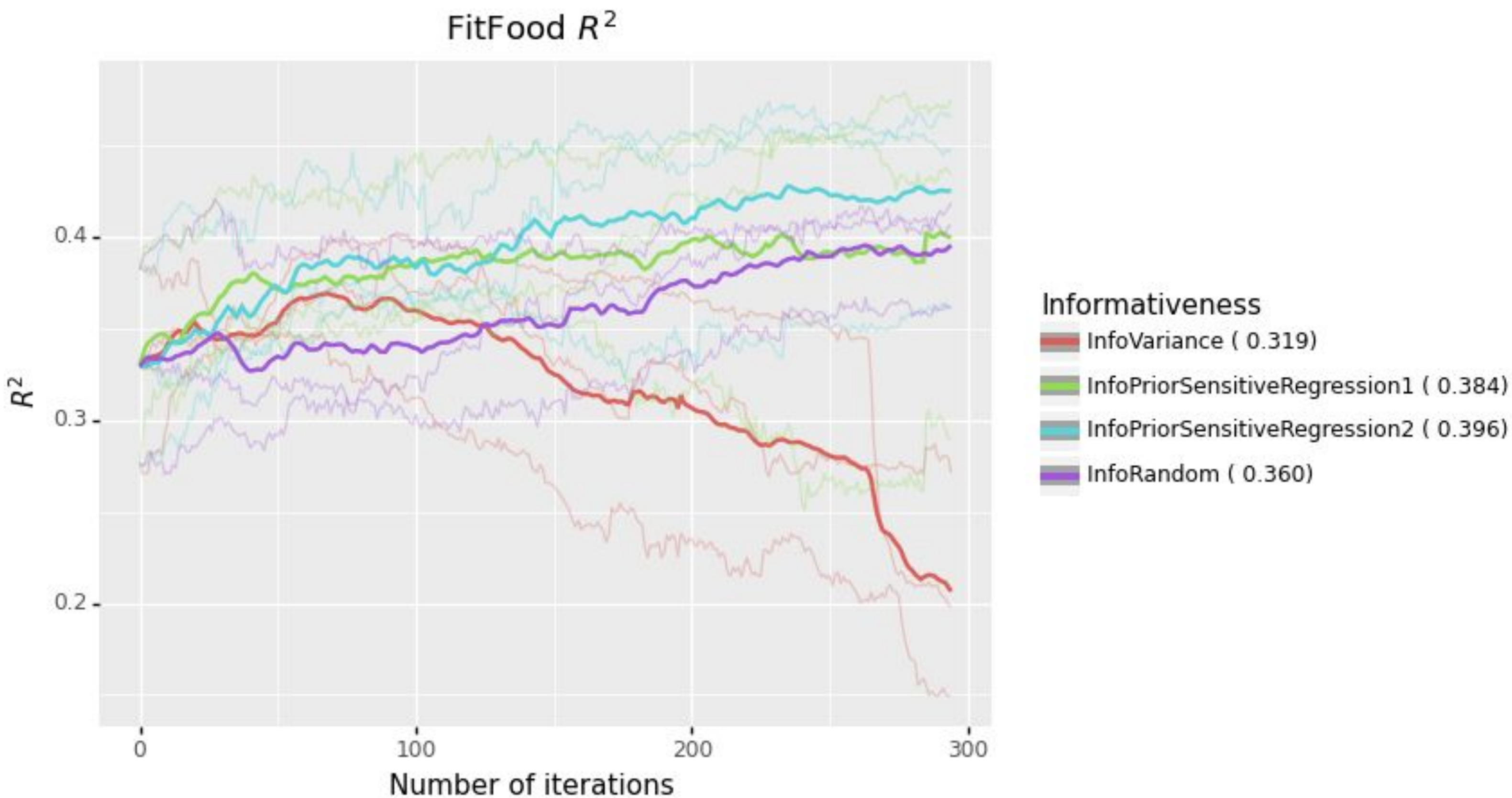


- Initial batch size: 200 (1% of the pool) and 200 iterations.
- XGBoost learner with default settings.

Regression uncertainty sampling

- Exemplary regression uncertainty sampling methods:
  - Variance-based: $u^*_{Var} = \arg\max_u Var(\Phi(u))$
  - Prior density-scaled: $u^*_{\mu} = \arg\max_u Var(\Phi(u)) \cdot \int_{E(\Phi(u))-\epsilon}^{E(\Phi(u))+\epsilon} \Phi(x)dx$
  - Differential entropy: $u^*_H = \arg\max_u \left(- \int \Phi(u)(x) \log \Phi(u)(x) dx \right)$
- Our model Φ needs to return distributions (not only the predictions)…
- **We may need to take into consideration the prior distribution of targets (*Φ*) - but how can we do that?!?**

An exemplary application - a regression task



- Initial batch size: 300 (1% of the pool), and 300 iterations.
- XGBoost trained using a natural gradient learner with a negative binomial prior.

Estimating the decision boundary

- Depending on the evaluation metric, it might be desirable to use a problem-specific decision boundary.
  - But we don’t have to many labels…
  - and we don’t want to do random sampling.
  - We may want to balance the predictions (e.g., to optimize the BAC metric).
- Instead of estimating the distribution of the target variable using known labels, **use the distribution of predictions**!
  - It works well for classification and regression problems.

Evaluation in active learning experiments

- We only simulate “real-life” problems.
- We don’t have to rely on real oracle - we have the labels.
  - We focus on testing the query selection methods…
  - or model updating techniques (more on this topic in future).
- The four main KPIs in active learning:
  - What performance level did we achieve after a fixed number of queries?
  - How many queries we needed to achieve the required performance level?
  - Area under the performance curve.
  - Stability of the model training process.

Summary

- We discussed the pool-based selective sampling approach to Active Learning.
- We focused on uncertainty sampling techniques.
- We discussed several uncertainty measures for classification and regression tasks which can be used to guide the AL process.
- We briefly talked about the performance evaluation in active learning experiments.
- We analyzed a few application examples for different ML tasks.

Literature:

1. B. Settles. Active Learning Literature Survey. Computer Sciences Technical Report 1648, University of Wisconsin–Madison, (2010).
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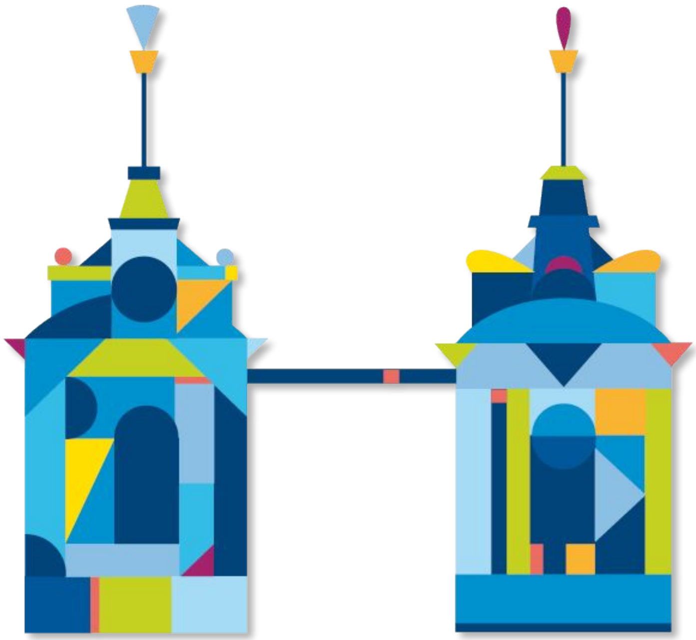

QUESTIONS OR COMMENTS?

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