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WYDZIAŁ MATEMATYKI, INFORMATYKI I MECHANIKI

Active Learning - the introduction

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THE PLAN

- Introduction
- Active Learning basics
- A discussion of various Active Learning scenarios
- A deeper dive into the membership query synthesis and stream-based selective sampling
- Exemplary algorithms and use-cases
- Summary

Active Learning

- Goal: obtain the best possible model with limited labeling capabilities, assuming that we can interact with the experts asking them to label indicated samples.
- How: iteratively query experts about labels for the most interesting/informative samples.
- Which samples are informative?
- Can we trust our experts?

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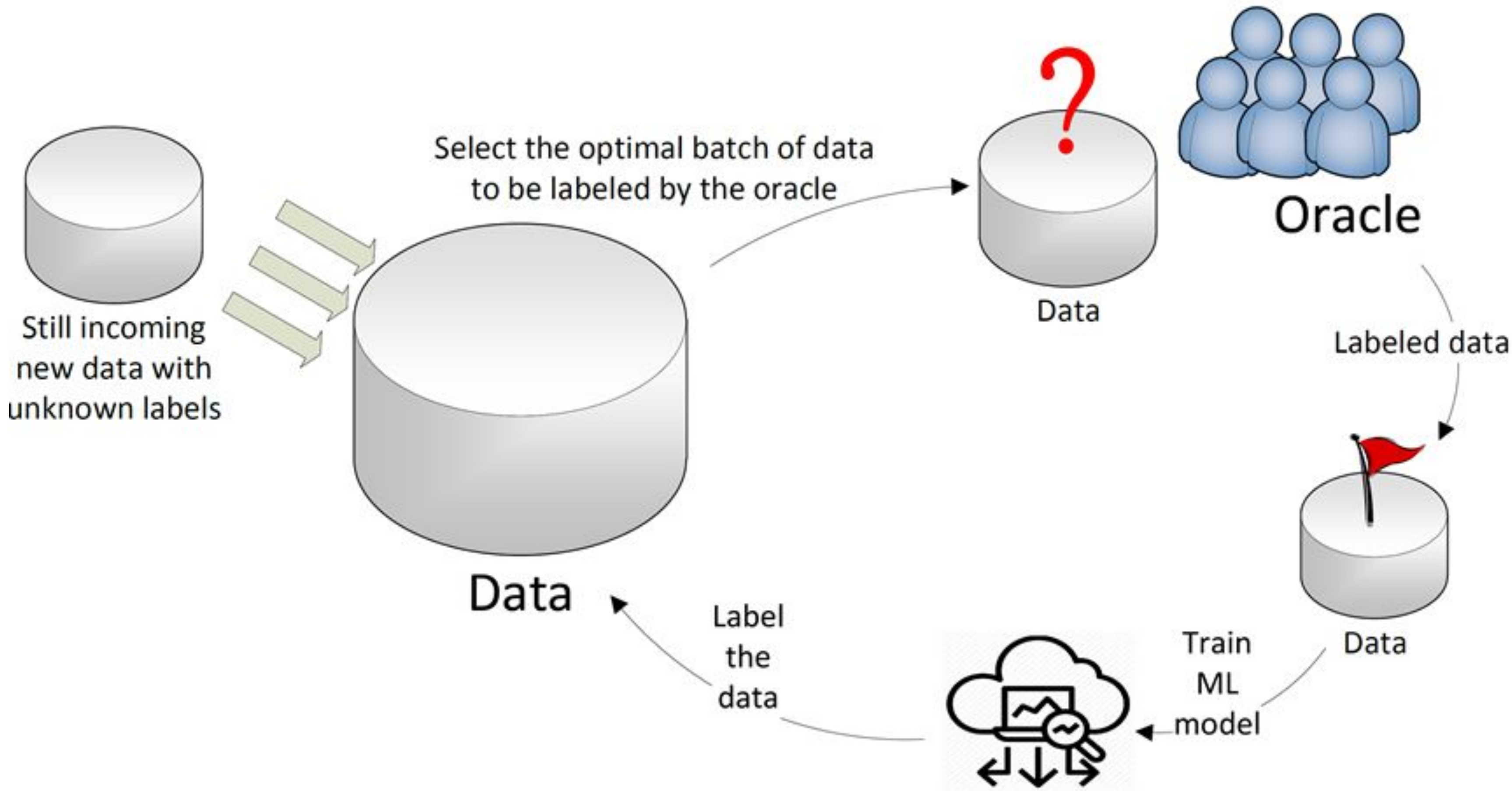
A glossary (simplified)

- Learner - typically, an ML model that we want to actively train to perform a given prediction task.
- An instance/case - an entity described in our data for which we are making predictions/decisions.
- A query - an instance that we send to the oracle to obtain the label.
- A sample - one or more data instances drawn from the data space.
- The oracle - typically, a committee of experts that can assign labels to data instances.
- Ground truth - the actual label that should be assigned to a data instance.

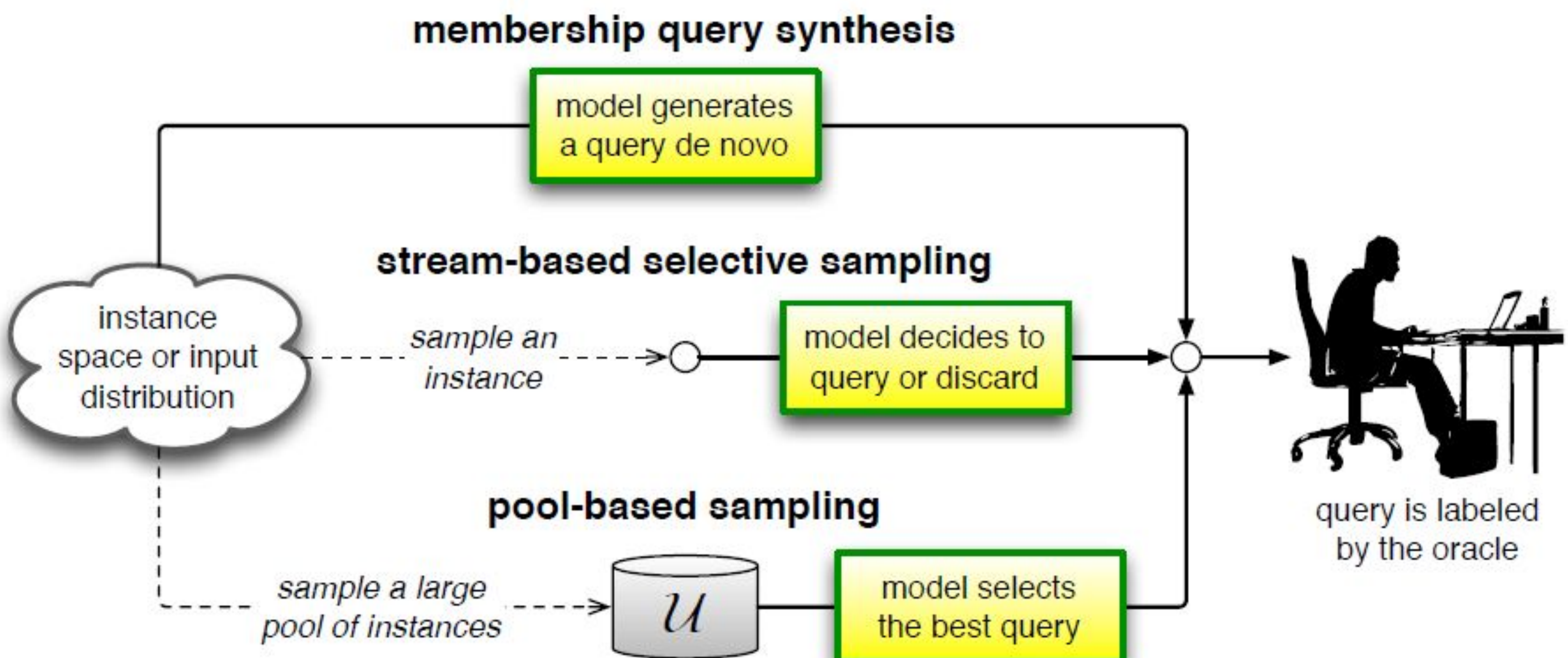
The active learning cycle



Exemplary application areas

- **Speech recognition:** It is extremely time-consuming and requires trained linguists. The annotation of speech recordings on a phoneme level can take 400 times longer than the actual recordings.
- **Natural language processing:** Many NLP-related ML tasks (information extraction, entity recognition, sentiment analysis) require detailed annotated data. The annotations/labels are often domain-specific and require expertise in a particular application field.
- **Image/video data processing:** Image classification, object detection or image segmentation require labeled examples. As with the NLP, in many domains (e.g., medicine) it requires specialized knowledge. Additionally, marking complex shapes is laborious.
- **Process mining:** Annotation of multivariate time series requires specialized tools, and if the data is multi-modal (e.g., video games data) the task is even more difficult.

The three main Active Learning scenarios



Schema from *Burr Settles: Active Learning Literature Survey (2010)*

Membership query synthesis

- One of the first Active Learning methods considered in ML literature.
- **The learner may request a label for any unlabeled instance in the input space, even if it is synthetic (not necessarily sampled from available data).**
- The generation of valid instances/queries might be problematic.
- Particularly effective in scenarios where the oracle is automatic (non-human), e.g., scientific experiments, computer simulations.

Speeding up simulations

- Membership query synthesis can be used to speed up scientific simulations.
  - We want to learn to predict experimental outcomes.
  - We can acquire some exemplary labels by performing costly or time-consuming experiments.
  - A reliable model would allow for tremendous efficiency improvements!
- How to synthesize a query?
  - Loss gradient-based optimization (if the model’s loss is smooth and differentiable with regard to the input).
  - Other optimization heuristics (e.g., hill climbing, simulated annealing, genetic algorithms).

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An exemplary application 1

- King et al. (2004) show an example of a successful application of the membership query synthesis strategy.
  - Experimental discovery of metabolic pathways in the yeast.
  - Experiments performed by a robot.
  - Instances - a mixture of chemical solutions (a growth medium, yeast mutant).
  - Labels - the experiment outcomes.
- The active learning approach resulted in 100-fold decrease in cost compared to randomly generated experiments and 3-fold decrease in comparison to the greedy sampling heuristic.

Image: Freepik.com

Selective sampling

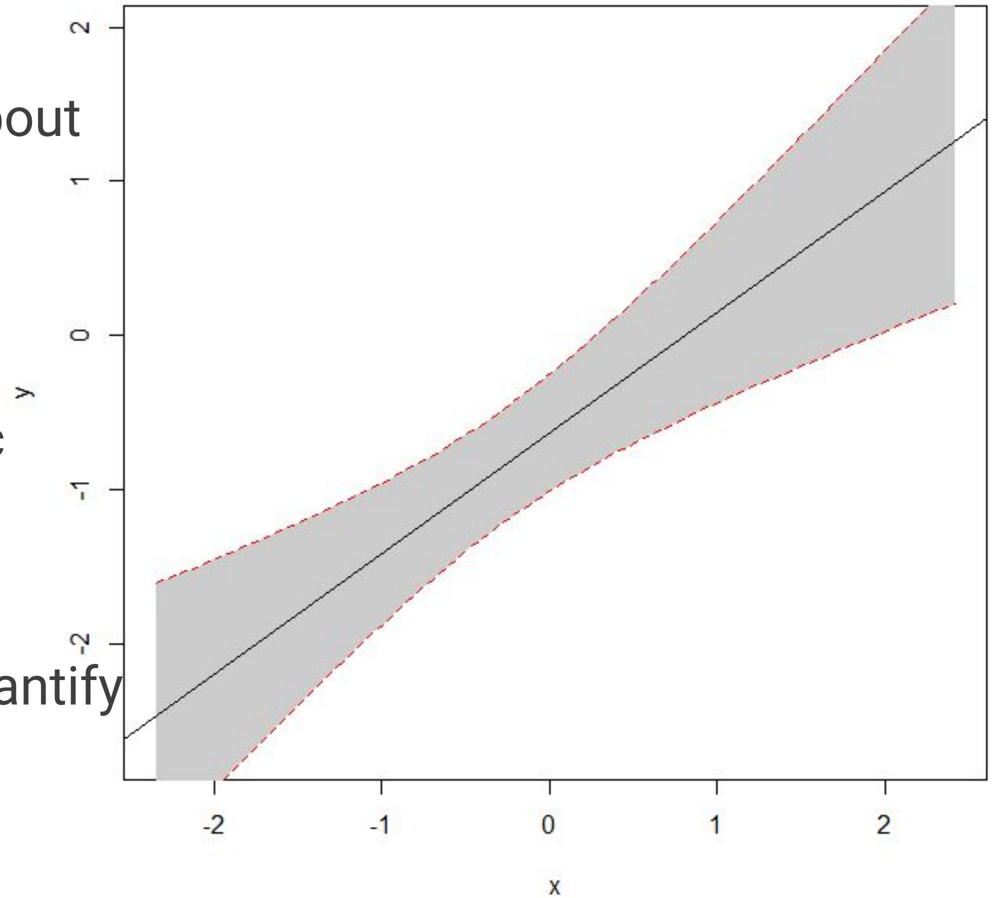
- Instead of synthesizing queries/instances, sample real cases from available examples.
  - No awkward or unrealistic cases which can be difficult to label by human annotators…
  - but the number of available examples needs to be large!
- Two main application scenarios:
  - Stream-based selective sampling.
  - Pool-based selective sampling.

Stream-based selective sampling

- Learner pulls out unlabeled instances one at a time from the data source.
  - For each instance, the learner has to decide whether to query the oracle for the label or discard it.
  - Even if the data distribution is not uniform, the sampled instances will reflect it.
- If the stream velocity is high, random sampling techniques are often used prior to the querying decision.
- The decision about the query is made based on the informativeness of an instance (e.g., the uncertainty of the learner).

Informativeness and uncertainty

- Informativeness of an instance expresses how much new information the knowledge about its label could provide to the learner.
- The informativeness is often associated with the epistemic uncertainty of a learner with regard to its predictions.
- In practice, we can usually quantify only the joint epistemic and aleatoric uncertainty.
- More details in the next lecture! 😊



Uncertainty-biased random sampling

- One of the simplest algorithms for selecting instances for querying.
- For any sampled instance *u*, the learner queries the oracle with a probability depending on the informativeness of *u*, e.g.:

$$P_{query}(u) = \frac{1}{1 + e^{\left(-\frac{Info(u)-\mu}{\sigma}\right)}} > rand(0,1)$$

- In practice, a possible informativeness function in this case is the Least Confidence uncertainty:

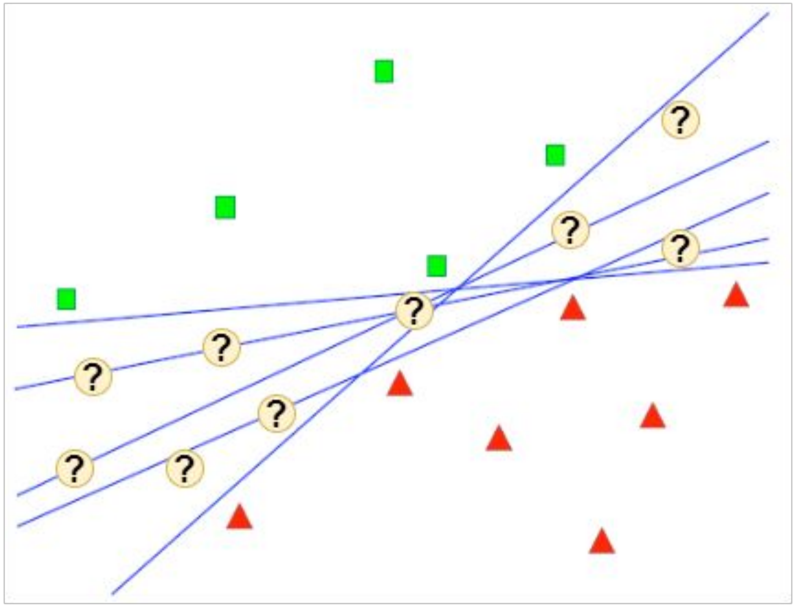
$$Info(u) = \frac{k\left(1 - P(y^*|u)\right)}{k-1}$$

Region of uncertainty querying

- Learner queries the oracle only if the sampled instance falls into learner's "*region of uncertainty*".
- How can we decide where exactly that region is?
  - We can set a specific threshold… (not so good idea).
  - We may try to decompose the data space into uncertainty regions using synthetic samples…
    (not so good idea either).
  - We can use a committee of prediction models!
    - The problem with this lies in the computational cost…
- The uncertainty region needs to be recalculated after each update of the learner.

The Query-By-Committee algorithm

- Proposed by Seung et al. (1992).
- The learner is composed of at least two prediction models of the same model class.
  - The models are sampled from, so-called, *version space*.
  - In computational learning theory, the version space is a set of hypotheses (models with different parametrization) that equally fit the training data but may disagree on new cases.
- An instance sampled from the stream is queried if the models sufficiently disagree.



Sampling from the version space?

- The main idea of the QBC algorithm is to query from the uncertainty region, thus limiting the “size” of the version space.
- It can be computationally challenging.
  - Typically, it is done approximately…
- For probabilistic (Bayesian) models, we may sample the parameter space.
- For other types of models, many ensemble learning techniques can be used:
  - Bootstrapping.
  - Segmentation of the feature space.

Disagreement in a committee

- We need to measure if the disagreement in the committee is sufficient to query the sample.
  - It is easy when there are only two models - in practice, it is often the case.
  - If there are many models, one may use the number of disagreeing pairs of voters.
  - Entropy of votes: $$\phi_{VE}(u) = -\sum_{l \in L} \frac{|\{i : y_i^* = l\}|}{K} \log\left(\frac{|\{i : y_i^* = l\}|}{K}\right)$$
  - Mean KL divergence: $$\phi_{KL}(u) = \frac{1}{K} \sum_{i=1}^{K} \sum_{l \in L} P_{\theta(i)}(y = l|u) \log\left(\frac{P_{\theta(i)}(y = l|u)}{P_{\Theta}(y = l|u)}\right)$$
- In the case of many voters, it is necessary to set a reasonable threshold - it may not be that easy.

An exemplary application 2

- Settles and Craven (2008) show an application of the QBC algorithm in the NLP domain.
  - Sequences of words -> streams of tokens.
  - The named entity recognition (NER) task on several different text corpora.
  - Instances - sequences of tokens (various length) with part-of-speech annotations.
  - Labels - the entity type associated with the sequence.
- The learners -> CRF models trained by bagging (an approximation of the version space).
  - Sequence vote entropy was proposed as the disagreement/uncertainty measure.

$$\phi_{SVE}(u) = -\sum_{l \in L^N} P_\Theta(y = l|u) \log(P_\Theta(y = l|u))$$

- The QBC algorithm performed consistently better than random and uncertainty samplings.

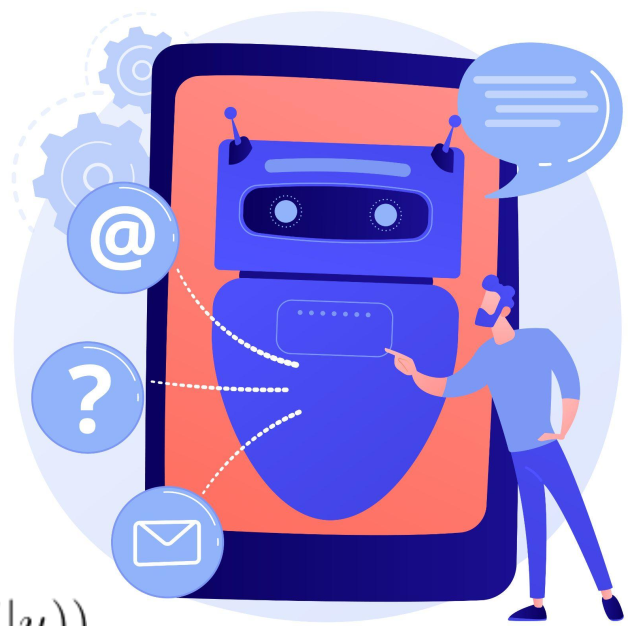
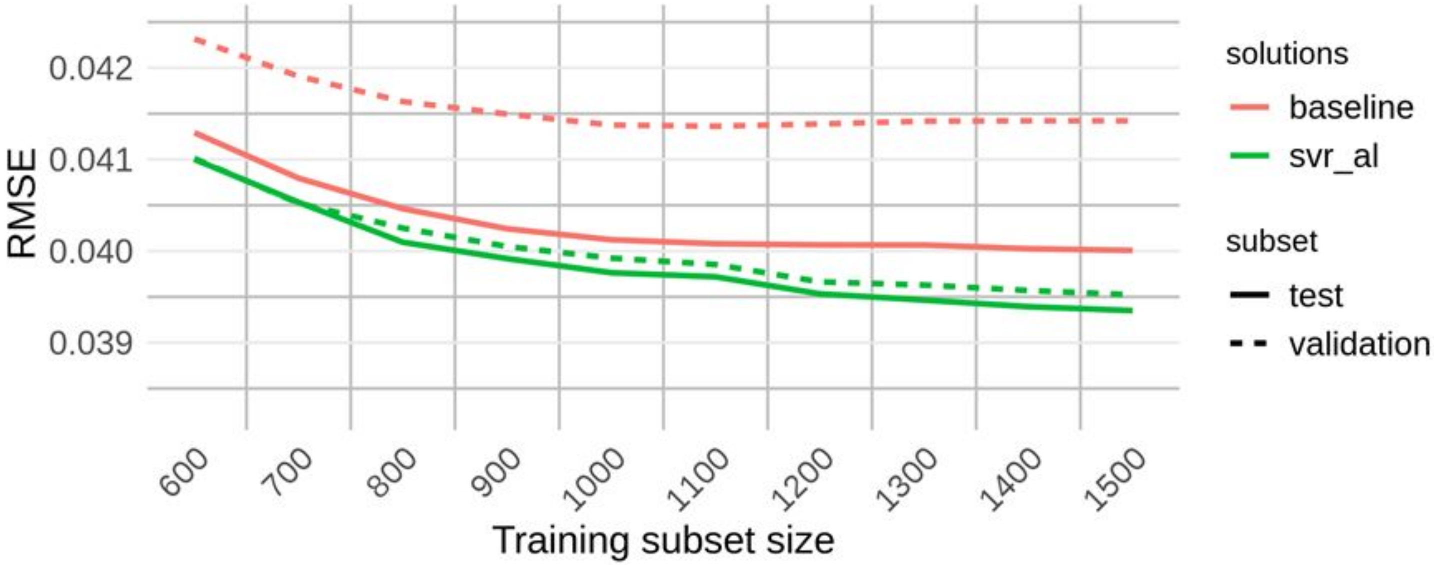


Image: Freepik.com

Pool-based selective sampling

- The <u>most common</u> active learning scenario.
  - Applicable when a large collection of unlabeled data is available.
  - At each iteration of the AL cycle, we may choose from many instances.
  - The unlabeled data pool may grow in time…
- An informativeness measure is used to evaluate all instances from the pool.
  - If the pool size is very large, some subsampling can be used…
- Queries are typically chosen in a greedy fashion.
- Numerous real-world applications!
- More about this approach in the next lecture ☺

An exemplary application 3



- 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/

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Summary

- We discussed the basic principles of active learning.
- We considered three different active learning application scenarios, with their pros and cons.
- We talked about the informativeness of instances in the context of AL and its relation to the uncertainty of the learner.
- We analyzed a few AL algorithms and application examples for different real-world ML tasks.

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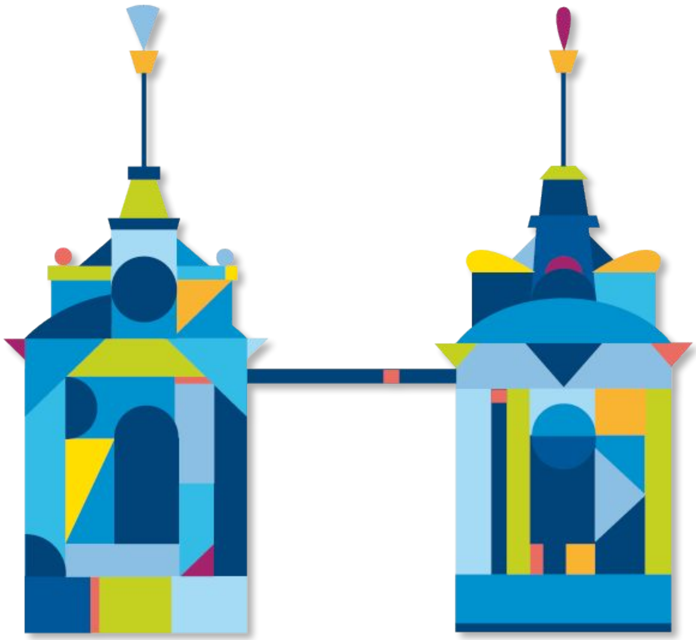

QUESTIONS OR COMMENTS?

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