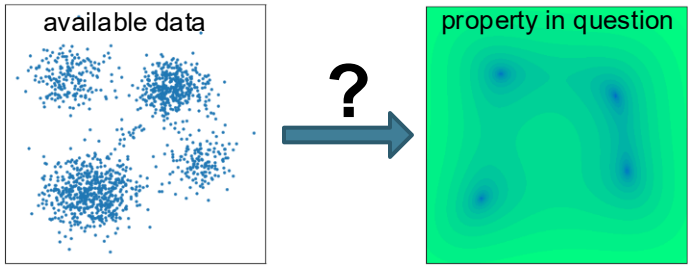
Liza Surzhikova (TU Brauschweig) | 06.11.2025

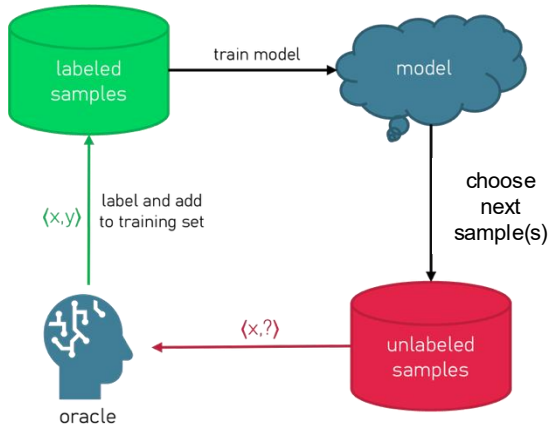
Active Learning

Assumption: Label generation most expensive step of training.
→ Learn property space with *as little labeled samples* as possible!

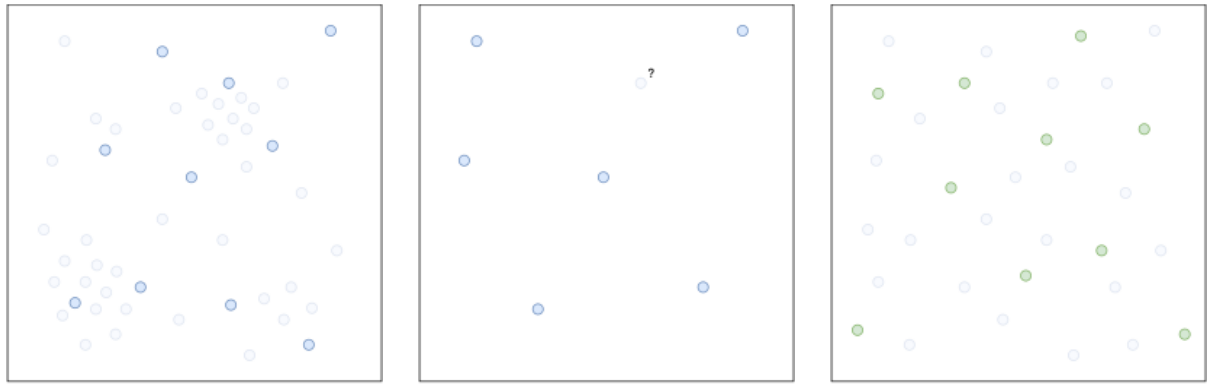


Active Learning

- iteratively develops training set with minimal labelling effort
- uses most informative available samples to avoid redundancy
- can pick one or batch of samples per iteration
- applicable to classification and regression problems

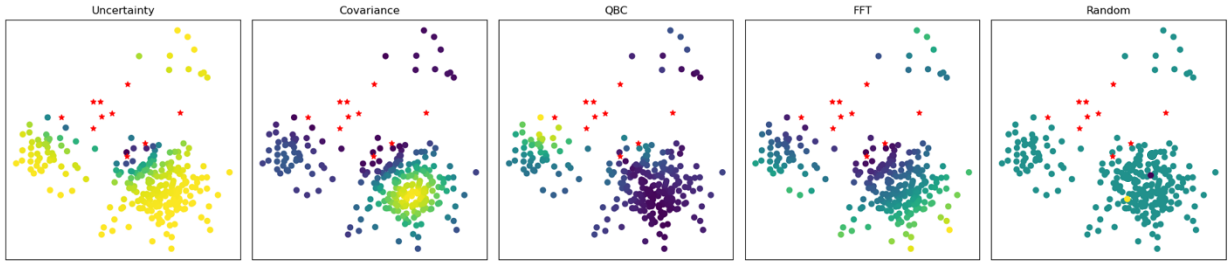


Pool-based setting | Stream-based setting | Synthetic setting

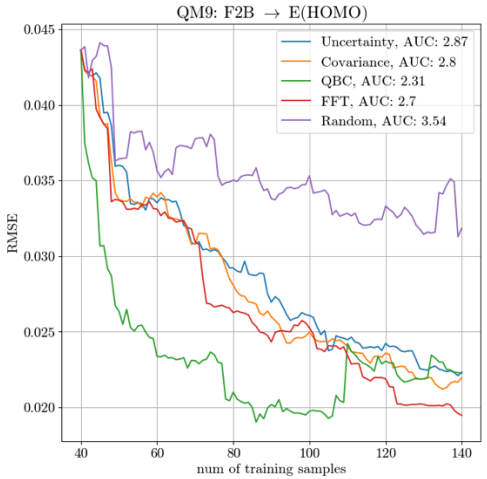


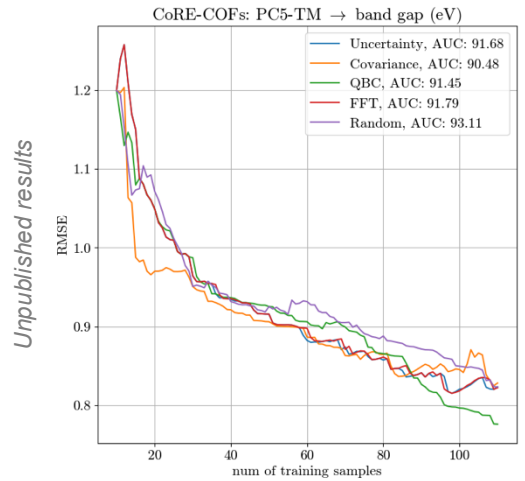
unlabeled sample | labeled sample | newly synthesized sample

Pool-based AL Strategies



Performance Examples





Applications in Chemistry

- Chemical space exploration
- Dataset reduction and/or construction
- Experiment prioritization

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