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WYDZIAŁ MATEMATYKI, INFORMATYKI I MECHANIKI

Active Learning - the pool-based selective sampling (part 3)

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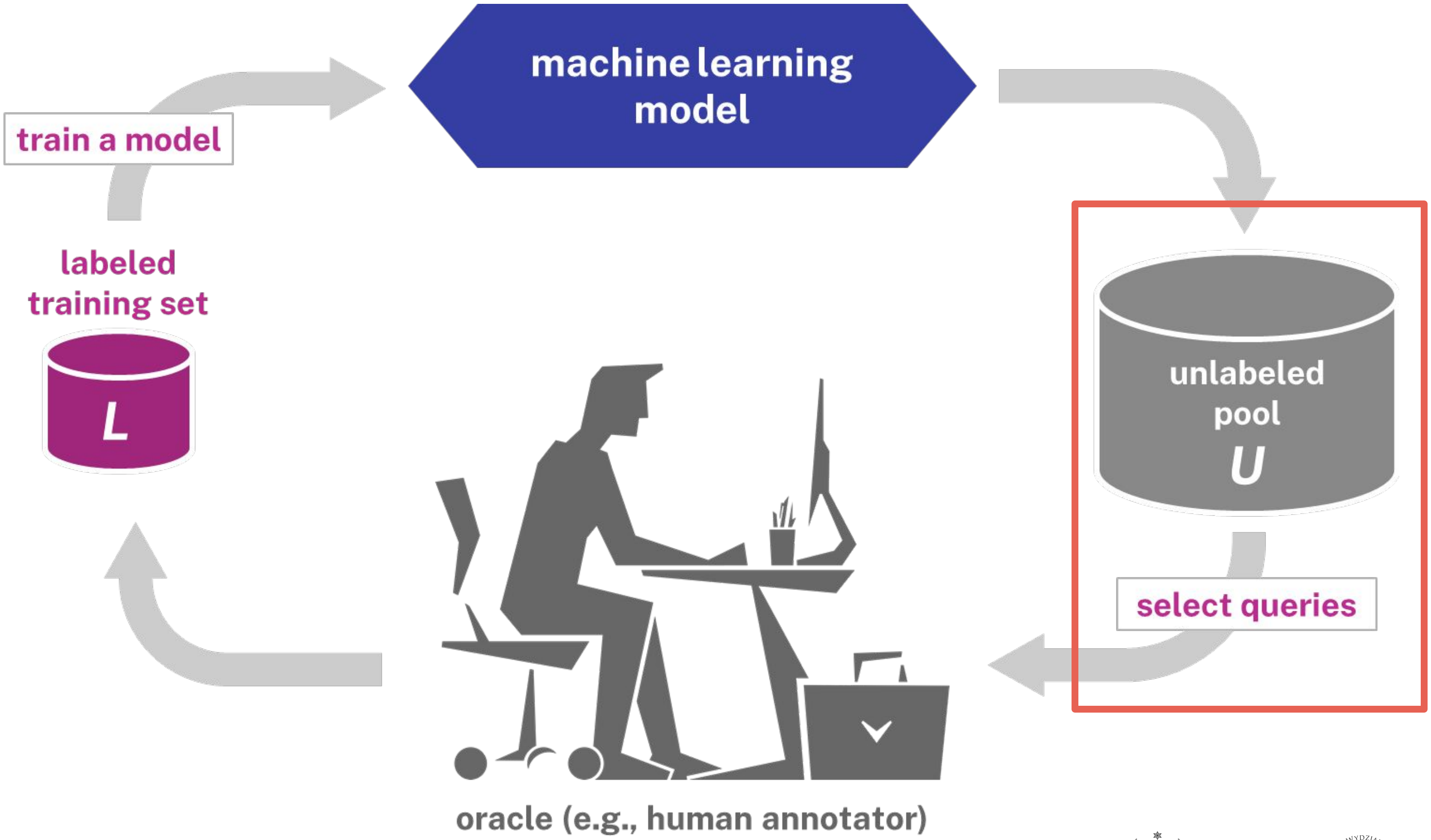
THE PLAN

- A recap of the previous lectures.
- Expected Model Change framework.
- Expected Error Reduction.
- Monte Carlo Dropout-based technique for training Bayesian neural networks.
- The BALD algorithm and decomposition of uncertainty.
- Exemplary algorithms and use-cases.
- Summary.

The active learning cycle - again



Uncertainty, representativeness, diversity

We search for a subset of data pool $U^* \subset DP$ that maximizes generalization capacity of our model:

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

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

We considered modeling the sample informativeness using the “uncertainty-representativeness-diversity” approach:

$$Info(u,B) = \frac{1}{c} \cdot Unc(u) + \left(\frac{1}{r} \cdot R(u)\right)^{\alpha} + \left(\frac{1}{d} \cdot Dis(u,B)\right)^{\beta}$$

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The initial data batch

- The initial batch has huge impact on the active learning performance.
  - Random sampling.
  - Iterative sampling using the representativeness-diversity function.
  - Clustering-based sampling.
- Regardless of the initial batch selection method, random samples are always needed for the evaluation!

A different view on the informativeness

- It is difficult to discern between aleatory and epistemic uncertainty.
- It might be difficult to tell which uncertainty function is the most suitable for a given model/task.
- We may try to take a more direct approach to the assessment of sample's usefulness.
  - Can we measure the impact of a sample on the training process?

Expected model change (EMC) framework

- Instead of measuring the prediction uncertainty, we may measure how the addition of a given sample to the labeled set *would change the model*.
  - We need to compute the expectation over all possible labelings.
  - May be computationally challenging.
- We quantify "*the change*" differently for different types of prediction models.
- Typically, this method is combined with gradient descent learning algorithms.

Gradient descent algorithm

- Gradient descent (GD) is a first-order optimization algorithm.
- Having defined a loss function, we iteratively search for the local minimum moving in the opposite direction to the gradient (the steepest descent).
- A common training algorithm for ML models:

$$\theta := \theta - \alpha \frac{\partial \ell_\theta(U_{tr})}{\partial \theta}$$

- Stochastic gradient descent (SGD) is a stochastic approximation of GD.

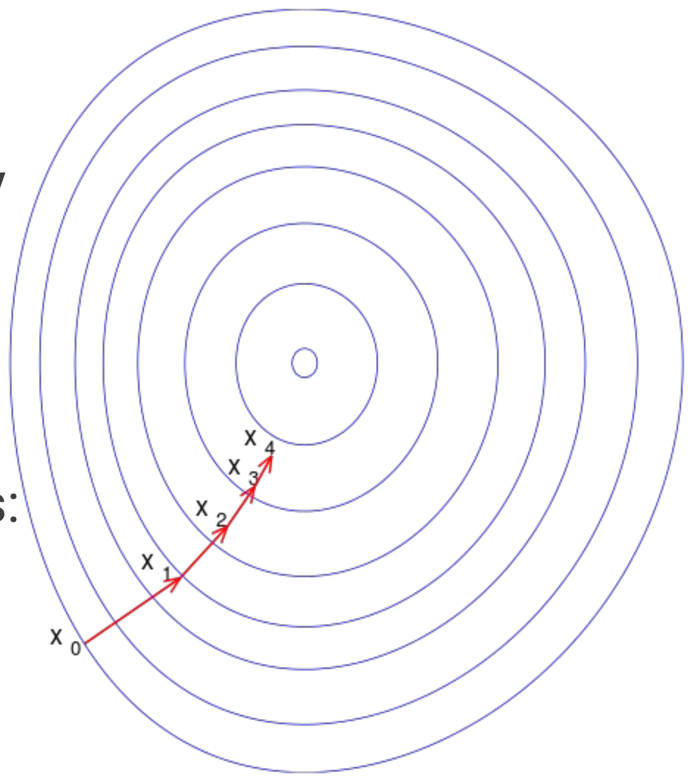

Image taken from Wikipedia (public domain).

Expected gradient length

- A special case of EMC for gradient-based learning algorithms.
- The "change" of the model corresponds to the length of the training gradient $\nabla \ell_\theta(U_{tr})$.
  - We query using the rule:

$$u^*_{EGL} = \arg\max_u \sum_i P(y_i|u)\, ||\nabla \ell_\theta(U_{tr} \cup \langle u, y_i \rangle)||$$

  - If we assume that samples are independent, we get:

$$u^*_{EGL} = \arg\max_u \sum_i P(y_i|u)\, ||\nabla \ell_\theta(\langle u, y_i \rangle)||$$

- Appropriate data scaling is a must!

An example - AL with linear regression

- W. Cai et al. (2013) demonstrate effectiveness of the EMC method for training linear regression model on several benchmark data sets.
- Bootstrapping of *K* models is used to estimate the distribution of predictions.
- For the typical squared error loss, the query selection rule simplifies to:

$$u^*_{EGL} = \arg\max_u \frac{1}{K} \sum_{k=1}^{K} ||(\Phi_k(u) - \Phi(u)) \cdot u||$$

- EMC outperformed the query-by-committee (QBC) and other baselines on all considered data sets.

***Concrete* data set from the UCI repository.**

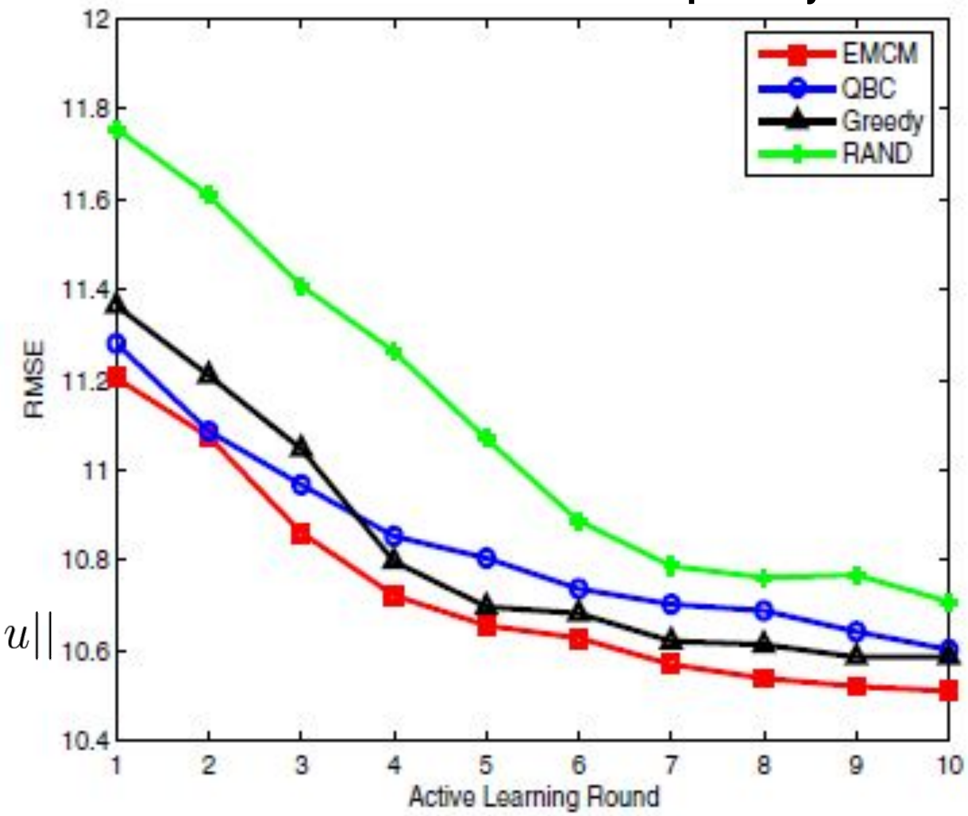

Image taken from W. Cai, et al. (2013), Maximizing Expected Model Change for Active Learning in Regression.

Expected error reduction (EER) approach

- A decision-theoretic framework aiming to measure how much model's generalization error is likely to be reduced by the information about the true label.
  - As in the case of EMC, we need to compute the expectation over all possible labels.
  - We assume that predictions of the new model are correct and estimate the generalization error on U.
  - Or we estimate the error using leave-one-out technique on the labeled data set U_{tr}.

EER for various losses

- We may select the query that minimizes the expected 0-1 loss:

$$u^*_{0-1} = \arg\min_{u \in U} \sum_i P_\theta(y_i|u) \left(\sum_{x \in U \setminus u} 1 - P_{\theta+(u,y_i)}(\hat{y}|x) \right)$$

- or the one that minimizes the expected log-loss:

$$u^*_{log} = \arg\min_{u \in U} \sum_i P_\theta(y_i|u) \left(-\sum_{x \in U \setminus u} \sum_j P_{\theta+(u,y_i)}(y_j|x) \log(P_{\theta+(u,y_i)}(y_j|x)) \right)$$

- In any case, the required computations might be prohibitive even for moderate-size data pools.

An example - Monte Carlo Estimation of EER

- In *N. Roy & A. MacCallum 2001*, authors propose a modification of the typical EER approach:

$$u^*_{EER} = \arg\min_{u \in U} \sum_i P_\theta(y_i|u) \left(\int_{x \in X \subset U} L(\hat{y}, P_{\theta+(u,y_i)}(y|x)) P(x) \right)$$

- The loss is estimated on a random subset of the unlabeled pool *U*.
- Incremental training instead of re-training the model from the scratch.
- Only a part of (similar) instances needs to be re-classified.
- Experiments with Naive Bayes and document classification.
- Good performance using four times less queries than considered baselines (QBC, uncertainty, random).

Variance reduction framework

- A direct minimization of the expected loss is usually extremely expensive computationally, and in general cannot be done in closed form.
- An indirect minimization of the expected loss is sometimes possible...
  - For a regression problem and the squared error loss:

$$
\begin{aligned}
E_U[(\hat{y} - y)^2 | u] &= E[(y - E[y|u])^2] && \text{model-independent} \\
&+ (E_{U_{tr}}[\hat{y}] - E[y|u])^2 && \text{model's bias} \\
&+ E_{U_{tr}}[(\hat{y} - E_{U_{tr}}[\hat{y}])^2] && \text{model's variance}
\end{aligned}
$$

Fisher information matrix

- By reducing the variance, we always reduce the generalization error.
- For some models (e.g. NN, LR, GMM), the variance of output can be easily estimated.
  - For a neural network and the squared error loss:

$$\sigma_{\hat{y}}^2 \approx \left[\frac{\partial \hat{y}}{\partial \theta}\right]^T \left[\frac{\partial^2}{\partial \theta} L_\theta(U_{tr})\right]^{-1} \left[\frac{\partial \hat{y}}{\partial \theta}\right] \approx \nabla u^T F^{-1} \nabla u$$

- In some cases model retraining is not necessary.
- Query: $u_{VR}^* = \arg\min_{u \in U} \left\langle \hat{\sigma}_{\hat{y}}^2 \right\rangle^{+u}$

Bayesian NNs and variational inference

- BNNs allow to express the uncertainty of predictions.
  - We assume that the model's weights are stochastic: $\theta \sim p(\theta)$
  - We train the model using the Bayesian inference.

$$p(\theta|U_{tr}) = \frac{p(Y_{tr}|U_{tr},\theta)p(\theta)}{\int p(Y_{tr}|U_{tr},\theta)p(\theta)\partial\theta} \propto p(Y_{tr}|U_{tr},\theta)p(\theta)$$

- This computation is intractable - we have to approximate:

$$p(y|u,U_{tr}) = \int p(y|u,\theta)p(\theta|U_{tr})\partial\theta$$

$$\approx \int p(y|u,\theta)q^*(\theta)\partial\theta \approx \frac{1}{T}\sum_{i=1}^{T} p(y|u,\hat{\theta}_i)$$

Monte Carlo dropout

- Gal & Ghahramani (2016b) show that random zeroing of weights before each layer of NN is equivalent to Bayesian approximation of the model's parameter distribution:

$$\theta \sim p(\theta | U_{tr}) \approx q^*(\theta) = W_i \cdot diag([z_{i,j}]_{j=1}^{K_i})$$

$$where\ z_{i,j} \sim Bernoulli(p_i)$$

  - Standard DNNs are easier to train than Bayesian equivalents.
  - We train the model using dropout layers and keep them active for the inference.
- It can be applied to a wide variety of model families.

The BALD algorithm

- Introduced by Houlsby et al. (2011) for GPC but can be applied for any Bayesian model.

  Predictive distribution: $p(y|u,\theta) \;\; where \; \theta \sim p(\theta|U_{tr})$

- We want to query the case that maximizes the decrease in expected posterior entropy of parameters:

$$u^* = \arg\max_u H(\theta|U_{tr}) - E_{y\sim p(y|u,\theta)}[H(\theta|y,u,U_{tr})]$$

  - This can be equivalently rewritten as:

$$u^*_{BALD} = \arg\max_u \underbrace{H(y|u,U_{tr})}_{\text{total prediction uncertainty}} - \underbrace{E_{\theta\sim p(\theta|U_{tr})}[H(y|u,\theta)]}_{\text{aleatoric uncertainty}}$$

BALD application example

- In Murray et al. (2021) authors show an interesting application of the BALD algorithm.
  - Unlike in a typical BNNs, weights are kept deterministic while the model's depth is assumed to be stochastic.
  - A categorical prior is placed over the model's depth distribution:

$$p(d) = Cat(d|\{\beta_i\}_{i=0}^{D})$$

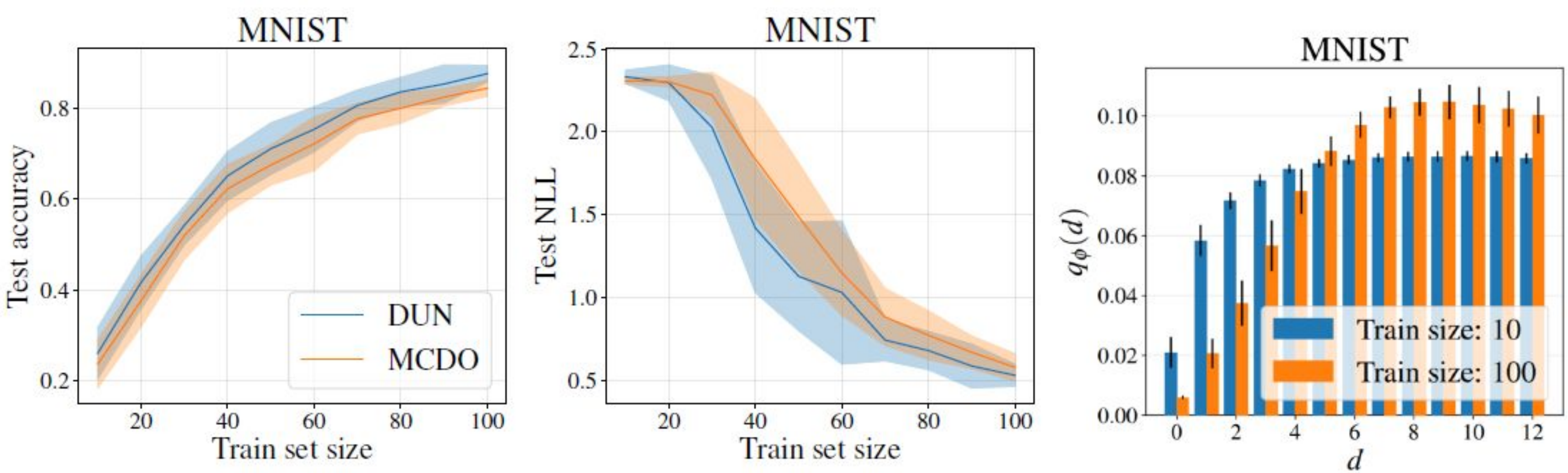

Image taken from Murray et al. (2021)

Pool-based selective sampling - summary (1)

- The most common AL scenario.
- A greedy selection of queries:
  - Uncertainty sampling.
  - Uncertainty-representativeness sampling.
- Diversification of query batches.
- Query-by-committee algorithm can be adapted to the pool-based scenario.

Pool-based selective sampling - summary (2)

- A different view of the uncertainty/informativeness of data samples:
  - How the sample's label would impact the model?
  - How much can we expect to reduce the model's error by querying for the sample's label?
- Decomposition of the model's uncertainty into the areatoric and epistemic parts.
  - The BALD approach to the uncertainty of Bayesian models.

Summary

- We discussed several methods for choosing the most informative samples in the pool-based selective sampling scenario.
- We considered variational inference and Bayesian neural networks for estimating the model's uncertainty.
- We talked about a decomposition of model's uncertainty into the aleatoric and epistemic parts.
- We analyzed a few AL algorithms and application examples for different ML tasks.

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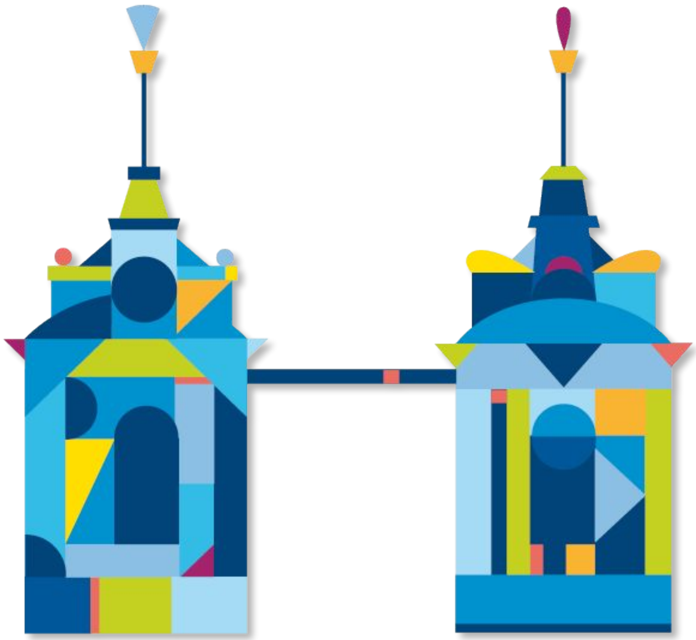

QUESTIONS OR COMMENTS?

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