Active Learning in Regression Tasks

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Selected Parts of Data Mining
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1 Introduction to Active Learning

- Motivation
- Active Learning Scenarios
- Uncertainty Sampling
- Version Space Reduction
- Variance Reduction

2 AL & Continuous Black-Box Optimization

- Motivation
- Bayesian Optimization
- Surrogate Models

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Active Learning in Regression Tasks
Bibliography

Motivation

Definition

**Active learning**

Machine learning algorithms that aim at reducing the training effort by posing queries to an oracle.

Targets tasks, in which:

- Unlabeled data are abundant
- Obtaining unlabeled instances is cheap
- Labeling is expensive
Introduction to Active Learning

Motivation

Examples of expensive labeling tasks

- Annotation of domain-specific data
- Extracting structured information from documents or multi-media
- Transcribing speech
- Testing scientific hypotheses
- Evaluating engineering designs by numerical simulations
- ...
Query Synthesis

- Learner may inquire about any instance from the input space
- May create uninterpretable queries
- Applicable for non-human oracles (e.g., scientific experiments)

(Lang and Baum, 1992)  
(King, 2004)
Selective (Stream-Based) Sampling

- Drawing (observing) instances from an input source
- The learner decides whether to discard or query the instance
- Applicable on sequential or large data
Pool-Based Sampling

- A small set $\mathcal{L}$ of labeled instances
- A large pool $\mathcal{U}$ of unlabeled instances
- Instances selected from $\mathcal{L}$ according to a utility measure evaluated on $\mathcal{U}$
- Most widely used in applications (information extraction, text classification, speech recognition, ...)
Pool-Based Uncertainty Sampling

1. $\mathcal{L}$ – initial set of labeled instances
2. $\mathcal{U}$ – pool of unlabeled instances
3. while true
   1. $\theta \leftarrow$ model trained on $\mathcal{L}$
   2. $x^* \leftarrow$ the most uncertain instance according to $\theta$
   3. $y^* \leftarrow$ label for $x^*$ from the oracle
   4. $\mathcal{L} \leftarrow \mathcal{L} \cup (x^*, y^*)$
   5. $\mathcal{U} \leftarrow \mathcal{U} \setminus (x^*)$
Uncertainty Measures – Least confident

\[ x_{LC}^* = \arg \min_x P_\theta(\hat{y}|x) \]
\[ = \arg \max_x 1 - P_\theta(\hat{y}|x) \]

- \( \hat{y} = \arg \max_y P_\theta(y|x) \)
- minimizes the expected zero-one loss
- Only the most likely prediction is considered
Uncertainty Measures – Margin

\[ x^*_M = \arg \min_x (P_\theta(\hat{y}_1|x) - P_\theta(\hat{y}_2|x)) \]
\[ = \arg \max_x (P_\theta(\hat{y}_2|x) - P_\theta(\hat{y}_1|x)) \]

- \( \hat{y}_1 \) and \( \hat{y}_2 \) – the first and second most likely classes, respectively
- Still ignores the remainder of the predictive distribution
Uncertainty Measures – Entropy

\[ x^*_H = \arg \max_x H(Y|x) \]
\[ = \arg \max_x - \sum_y P_\theta(y|x) \log P_\theta(y|x) \]

- Maximizes the expected log-loss
- Shannon entropy \( H \) – the expected self-information of a random variable
Uncertainty Measures

least confident
margin
entropy

Ternary distributions
Uncertainty Sampling in Regression

- Normal distribution maximizes entropy given a variance.
- Variance-based uncertainty sampling equivalent to entropy-based sampling under assumption of normality.
- Requires estimation of variance.

Variance-based sampling for a 2-layer perceptron

(Settles, 2012)
Uncertainty Sampling Caveats

- Utility measures based on a single hypothesis
- Training set \( \mathcal{L} \) is very small
- As a result, sampling bias is introduced

(a) target function  (b) initial sample  (c) uncertainty-based selective sampling over time

(Settles, 2012)
Version Space

- Hypothesis $H$ – a concrete model parametrization
- Hypothesis space $\mathcal{H}$ – the set of all hypotheses allowed by the model class
- Version space $\mathcal{V} \subseteq \mathcal{H}$ – the set of all hypotheses consistent with data
- Active learning → try to reduce $\mathcal{V}$ as quickly as possible

(Settles, 2012)
Query by Disagreement

1. $\mathcal{V} \subseteq \mathcal{H}$ – the version and hypothesis spaces, resp.
2. $\mathcal{L}$ – the initial set of labeled instances
3. repeat
   1. receive $x \sim \mathcal{X}$ {the stream scenario}
   2. if $\exists h_1, h_2 \in \mathcal{V}, h_1(x) \neq h_2(x)$ then
      - query label $y$ for $x$
      - $\mathcal{L} \leftarrow \mathcal{L} \cup (x, y)$
      - $\mathcal{V} \leftarrow \{h : h \text{ consistent with } \mathcal{L}\}$
   3. else
      - discard $x$
4. return $\mathcal{L}$
Practical Query by Disagreement

Version space $\mathcal{V}$ might be uncountable and thus unrepresentable

- Speculative hypotheses approach
  - $h_1 \leftarrow \text{train}(\mathcal{L} \cup (\mathbf{x}, \oplus))$
  - $h_2 \leftarrow \text{train}(\mathcal{L} \cup (\mathbf{x}, \ominus))$

- Specific-General ($SG$) approach
  - A conservative $h_S$ and a liberal $h_G$ hypothesis
  - Approximation of region of disagreement by $\text{DIS}(\mathcal{V}) \approx \{\mathbf{x} \in \mathcal{X} : h_S(\mathbf{x}) \neq h_G(\mathbf{x})\}$
  - Obtaining $h_S$ and $h_G$: assign $\oplus$ and $\ominus$, in turn, to a sample of background points $\mathcal{B} \subseteq \mathcal{U}$
Query by Disagreement – Example

(f) disagreement-based selective sampling over time

(g) uncertainty-based selective sampling over time

(Settles, 2012)
Previous heuristics were not aimed at predictive accuracy

The goal: select points that minimize the *future* expected error

Equivalent to reducing output variance (Geman et al., 1992):

$$x_{VR}^* = \arg \min_{x \in \mathcal{L}} \sum_{x' \in \mathcal{U}} \text{Var}_{\theta^+}(Y|x')$$

- $\theta^+$ – model after retraining on $\mathcal{L} \cup (x, y)$

A straightforward implementation leads to complexity explosion
Score

Given a model of random variable $Y$ with parameters $\theta$, the score is the gradient of the log likelihood w. r. t. $\theta$:

$$u_\theta(x) = \nabla_\theta \log L(Y|x; \theta)$$

$$= \frac{\partial}{\partial \theta} \log P_\theta(Y|x)$$
Fisher information is the variance of the score

\[ F(\theta) = \text{Var}(u_{\theta}(x)). \]

Under some mild assumptions, \( E[u_{\theta}(x)] = 0 \). Further, it can be shown:

\[
F(\theta) = E \left[ \left( \frac{\partial}{\partial \theta} \log P_{\theta}(Y|x) \right)^2 \right] \\
= -E \left[ \frac{\partial^2}{\partial \theta^2} \log P_{\theta}(Y|x) \right]
\]

- Expected value of negative Hessian matrix of log likelihood
- Expresses the amount of sensitivity of log likelihood w.r.t. to changes in \( \theta \)
Optimal Experimental Design

Cramér–Rao bound

\[ F(\theta)^{-1} \] is a lower bound on the variance of any unbiased estimator \( \hat{\theta} \) of parameters \( \theta \).

- “Minimize” Fisher information matrix inverse
- In general, \( F \) is a covariance matrix – what to optimize?
- Optimal Experimental Design (Fedorov, 1972) – strategies of optimizing real-valued statistics of Fisher information
- Using Fisher information, \( \text{Var}_{\theta^+}(Y|x) \) can be estimated without retraining at each \( x \)
D-Optimal Design

\[ \mathbf{x}_D^* = \arg \min_{\mathbf{x}} \det \left( (F_L + u_\theta(\mathbf{x})u_\theta(\mathbf{x})^T)^{-1} \right) \]

- Can be viewed as a version space reduction strategy
- Reduces the amount of uncertainty in the parameter estimates
A-Optimal Design

\[ \mathbf{x}_A^* = \arg \min_{\mathbf{x}} \text{tr}(AF_L^{-1}) \]

- \( A \) – a reference matrix
- Using \( A_{\mathbf{x}} = u_\theta(\mathbf{x})u_\theta(\mathbf{x})^T \) as the reference matrix leads to a variance sampling strategy

\[ \text{tr}(A_{\mathbf{x}}F_L^{-1}) = u_\theta(\mathbf{x})^TF_L^{-1}u_\theta(\mathbf{x}) \]

- Minimizes the average variance of the parameter estimates
Fisher information ratio

\[ x_{\text{FIR}}^* = \arg \min_x \sum_{x' \in \mathcal{U}} \text{Var}_{\theta^+}(Y | x') \]

\[ = \arg \min_x \sum_{x' \in \mathcal{U}} \text{tr} \left( A_{x'} \left( F_\mathcal{L} + u_\theta(x) u_\theta(x)^T \right)^{-1} \right) \]

\[ = \arg \min_x \text{tr} \left( F_\mathcal{U} \left( F_\mathcal{L} + u_\theta(x) u_\theta(x)^T \right)^{-1} \right) \]

- \( A_{x'} = u_\theta(x') u_\theta(x')^T \)

- Indirectly reduces the future output variance after labeling \( x \)
Comparison of Reviewed Strategies (Settles, 2012)

Uncertainty sampling
+ simple, fast
- myopic, might be overly confident about incorrect predictions

Query by committee / disagreement
+ usable with any learning algorithm, some theoretical guarantees
- difficult to train multiple hypotheses, does not try to reduce the expected error

Error / variance reduction
+ optimizes the objection of interest, empirically successful
- computationally expensive, difficult to implement
Definition

Optimize $f : \mathcal{X} \rightarrow \mathbb{R}$ on compact $\mathcal{X} \subseteq \mathbb{R}^D$

$$x^* = \arg \min_{x \in \mathcal{X}} f(x),$$

under conditions

- Unknown analytical definition of $f$
- Unknown (analytical) derivatives, continuity, convexity properties
- $f$ considered expensive to evaluate
- Observations of $f$-values possibly noisy
Motivation

Optimization of

- Empirical functions: material science, chemistry, ...
- Numerically simulated functions: engineering design optimization

Example: Photonic coupler design

(Bekasiewicz and Koziel, 2017)
\[ f - \text{the objective function} \]
\[ \mathcal{A} - \text{initial set of labeled instances} \]
\[ \textbf{repeat} \]
\[ \hat{f} \leftarrow \text{build the acquisition function on } \mathcal{A} \]
\[ x^* \leftarrow \arg\min_x \hat{f} \{ \text{optimize } \hat{f} \} \]
\[ y \leftarrow f(x^*) \{ \text{expensive evaluation} \} \]
\[ \mathcal{A} \leftarrow \mathcal{A} \cup (x^*, y) \]
Acquisition Functions

Lower Confidence Bound:

$$\text{LCB}(x) = \hat{f}(x) - \alpha \text{Var}(Y|X)$$

Probability of Improvement

$$\text{POI}(x) = P_Y(f(x) \leq T)$$

Expected Improvement

$$\text{EI}(x) = E \left( \max \{ y_{\text{min}} - f(x), 0 \} \right)$$
Evolution Strategies

- Population-based randomized search using operators of *selection*, *mutation* and *recombination*
- Covariance Matrix Adaptation Evolution Strategy – one of the most successful continuous black-box optimizer
  - Derandomized mutative parameters
  - Invariant towards rigid transformations of the input space
  - Invariant towards strictly monotonic transformations of the output space
$(\mu, \lambda)$-CMA-ES (Hansen, 2001)
Surrogate modeling

- Stochastic optimization still requires large no. of function evaluations
- Surrogate models of the objective can be utilized as a heuristic
- Two levels of evolution control (EC) are distinguished (Jin, 2002)
  - Generation-based – a fraction of populations is wholly evaluated with the objective function
  - Individual-based – a fraction of each population is evaluated with the objective function
Evolution Control

Generation-based EC

Individual-based EC

Objective function
Surrogate model

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Active Learning in Individual-Based EC

Given an extended population and a surrogate model of the objective function

- Select the most promising points
  - Combine optimality w. r. t. to the objective and utility for improving the model
- The same functions as in Bayesian optimization may be used
  - Lower confidence bound
  - Probability of improvement
  - Expected improvement
Example – Metamodelling Assisted Evolution Strategy
(Emmerich, 2002)

1. pop – an initial population
2. $f$ – the objective function
3. $C$ – a pre-selection criterion
4. $\mu$ – parent number
5. $\lambda, \lambda_{\text{Pre}}$ – population number, extended pop. number
6. repeat

   1. offspring ← reproduce(pop)
   2. offspring ← mutate(pop)
   3. offspring ← select $\lambda$ best according to $C$
   4. pop ← select $\mu$ best according to $f$
Experimental comparison

Selected model-based optimizers and CMA-ES compared on the Black-Box optimization benchmarking framework

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Further Reading I


Further Reading II


Thank you!
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