PyRelationAL: A Library for Active Learning Research and Development

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Abstract

In constrained real-world scenarios where it is challenging or costly to generate data, disciplined methods for acquiring informative new data points are of fundamental importance for the efficient training of machine learning (ML) models. Active learning (AL) is a subfield of ML focused on the development of methods to iteratively and economically acquire data through strategically querying new data points that are the most useful for a particular task. Here, we introduce PyRelationAL, an open source library for AL research. We describe a modular toolkit that is compatible with diverse ML frameworks (e.g. PyTorch, Scikit-Learn, TensorFlow, JAX). Furthermore, to help accelerate research and development in the field, the library implements a number of published methods and provides API access to wide-ranging benchmark datasets and AL task configurations based on existing literature. The library is supplemented by an expansive set of tutorials, demos, and documentation to help users get started. We perform experiments on the PyRelationAL collection of benchmark datasets and showcase the considerable economies that AL can provide. PyRelationAL is maintained using modern software engineering practices — with an inclusive contributor code of conduct — to promote long term library quality and utilisation.

1 Introduction

Machine learning (ML) models, particularly those using deep learning, play an increasing role in modern scientific research and broader society due to strong performance across tasks and domains. However, the success of such learning algorithms has often been fueled by large annotated datasets and well designed inductive biases. Unfortunately, many important domains — such as chemistry, biology, and medicine — operate in low data regimes [1], wherein the amount of data is relatively small compared to the rich and complex representations of each entity of interest. This problem can be attributed to the staggering cost and resources required to label a sufficient number of entities for effective learning [2, 3, 4]. For instance, labelling all pairwise combinations of the ∼4,000 FDA-approved drugs for synergistic effects at a single dose pair would require ∼8 million experiments per...

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phenotypic readout; this would require specialized equipment and could reasonably be considered experimentally infeasible.

Active learning (AL) is a machine learning paradigm where the aim is to develop methods, or strategies, to improve model performance in a data-efficient manner. Intuitively, an AL strategy seeks to sample data points economically such that the resulting model performs as well as possible under budget constraints. This is typically achieved via an interactive process whereby the model can sequentially query samples based on current knowledge and uncertainties. AL is also known as query learning in the computational learning theory literature [5] and is a concept that has come in and out of focus over the last decades. Notions in AL can be related to research in Bayesian optimization [6] and reinforcement learning [7], both aiming to strategically explore some space to improve on a performance metric. Recently, there has been a renewed interest in AL, especially in combination with advances in deep learning, to address various real-world applications [8, 9]. Notably, applications in medicine have seen growing interest both from academic and industrial institutes [2, 3, 10, 11, 12].

Here, we introduce PyRelationAL, an open source Python library for the rapid, reliable and reproducible construction of AL pipelines and strategies. The design is modular and allows easy implementation of AL strategies within a consistent framework. PyRelationAL enables the reproduction of existing research, the application to new domains, and the design of new methods. We include a plethora of published methods as part of PyRelationAL to help users get started and facilitate development around popular state of the art methods. Historically, the open source ML libraries that have played a major role in the fast paced advancement of ML have adopted a practical researcher-first ethos coupled with flexible design principles [13, 14, 15, 16, 17, 18, 19]. Our intention is for PyRelationAL to have a similar transformative impact for AL research.

We summarise PyRelationAL’s main contributions as follows:

- A modular toolkit to rapidly construct AL pipelines and strategies.
- A first-party interface to various popular ML frameworks through our generic ML manager (e.g. PyTorch, Sci-kit Learn, JAX, TensorFlow).
- Implementation of existing AL strategies for reproduction, modification and extensions.
- Collection of synthetic and real world benchmark datasets and AL task configurations for evaluating AL strategies horizontally across domains [9, 20, 21].

2 Active learning primer

Notations

Let $\mathcal{X}$ denote a state space whereby each element $x \in \mathcal{X}$ can be associated to a label $y \in \mathcal{Y}$. We further denote by $\mathcal{F}$ the space of functions mapping $f : \mathcal{X} \rightarrow \mathcal{Y}$. For a given ML architecture, we denote by $\mathcal{F}_\Theta \subset \mathcal{F}$ the subset of function mappings having this architecture and parameters in $\Theta$, which is defined by the model’s hyperparameters. The world, $\mathcal{W} \subset \mathcal{X} \times \mathcal{Y}$, is defined by a canonical mapping $\omega \in \mathcal{F}$ that associates to each state a unique label. We assume we have initially access to a set of observations $\mathcal{L}_0 \subset \mathcal{W}$ from the world. We denote by $\mathcal{U}_0 \subset \mathcal{X}$ the set of elements that are not observed in $\mathcal{L}_0$. The task we are faced with is to approximate the canonical mapping function $\omega$ from a subset of observations of $\mathcal{W}$, i.e. find $f \in \mathcal{F}$ such that $\forall x \in \mathcal{X}, f(x) \approx \omega(x)$.

| Symbol | Description |
|--------|-------------|
| $\mathcal{X}$ | Complete state space |
| $\mathcal{Y}$ | Corresponding label space |
| $\mathcal{F}$ | Space of functions mapping $f : \mathcal{X} \rightarrow \mathcal{Y}$ |
| $\omega : \mathcal{X} \rightarrow \mathcal{Y}$ | Canonical map we wish to learn |
| $\mathcal{F}_\Theta \subset \mathcal{F}$ | Subset of $\mathcal{F}$ representable using chosen numerical method |
| $\mathcal{W} \subset \mathcal{X} \times \mathcal{Y}$ | The world defined as a state-label pairing |
| $\mathcal{L}_k \subset \mathcal{W}$ | Observations at round $k$ |
| $\mathcal{U}_k \subset \mathcal{X}$ | Unlabelled samples at round $k$. |
Supervised learning  To address this task in the supervised ML paradigm, one first defines a function space $F_{\Theta}$, through various inductive biases and hyperparameter tuning. Then one typically searches for a function $f_{\hat{\theta}} \in F_{\Theta}$, with parameters $\hat{\theta} \in \Theta$, that best approximate $\omega$.

Active learning  In contrast, in the AL paradigm the function space $F_{\Theta}$ is largely assumed to be fixed, but the practitioner can iteratively increase the size of the dataset by strategically querying the labels for some unlabelled elements in $\mathcal{X}$. At the $k^{th}$ iteration, we denote by $\mathcal{L}_k$ the dataset and by $\mathcal{U}_k$ the set of unlabelled elements. The goal of an AL strategy is to identify a query set $Q_k \subseteq \mathcal{U}_k$ that carries the most information for approximating $\omega$. In other words, the AL practitioner looks to add new observations strategically to identify a smaller space $F_{\Theta,k} + 1$ of functions that are compatible with $L_{k+1} = L_k \cup \{(q, \omega(q)), q \in Q_k\}$, whereby the queries’ labels are provided by an oracle, e.g. human annotators or laboratory experiments. We then update $\mathcal{U}_{k+1} = \mathcal{U}_k \setminus Q_k$ for the next iteration.

The general framing described above, and illustrated in Figure 1, is sometimes referred to as pool-based AL [5], where $\mathcal{U}_k$ defines the pool at the $k^{th}$ iteration. This is arguably the most common framing of the AL problem. However, there exist variations whereby at each iteration $\mathcal{U}_k$ is not a finite set but either a generative process or a stream of unlabelled observation. These are known as membership query and stream based AL, respectively [5]. All framings share the same core problem: identifying unlabelled observations that are most informative to improving our solution to the task. In our exposition, we will principally focus on pool-based AL unless otherwise specified.

A critical question underpinning AL is how to measure the informativeness of each state in $\mathcal{X}$. A number of heuristics have been proposed in the past which can broadly be split into two categories: 1.) uncertainty-based category and 2.) diversity-based category. These are not mutually exclusive as the two notions can be combined to positive effect [5,22,23]. The former relies on some measure of uncertainties of the predictions obtained from the set of functions $F_{\Theta,k}$ at each iteration. In practice, $F_{\Theta,k}$ can be defined intrinsically by the class of ML models (e.g. Gaussian processes or Bayesian neural networks) or a subset of it can be obtained using heuristics such as ensembling [24,25,26] or Bayesian inference approximation methods like MCDropout [27]. Various informativeness scores can be computed from the uncertainty estimates (see Table 3) and used to select the query set $Q_k$.

In contrast, diversity-based heuristics rely on a distance measure $d : \mathcal{X} \times \mathcal{X} \mapsto \mathbb{R}_+$, which can depend on $F_{\Theta,k}$, to score states in $\mathcal{U}_k$ with respect to elements in $\mathcal{L}_k$. The choice of informativeness measure is an important challenge of AL as well as the choice of query selection strategy from the informativeness scores.

Figure 1: Generic pipeline for pool based AL scenarios following notations introduced in Section 2. The solid lines indicate the internal operations within an AL iteration. In practice the constrain operation is done through training the model(s) on $\mathcal{L}_k$. The optional dependency of the informativeness scoring on $F_{\Theta,k}$ is represented by the dotted line. The dashed line represents the update step based on external information provided by the oracle. The colors indicate the correspondence with the different modules in PyRelationAL: the data manager handling label tracking and updating, the model manager handling training and uncertainty estimation, and the AL strategy defining the informativeness measure and selection criteria. These components are detailed in Section 4.
A standard approach to select $Q_k$ is to greedily pick the highest scoring elements such that

$$Q_k = \arg\max_{Q \subseteq U_k, |Q| = m_k} \sum_{q \in Q} I(q),$$

where $I : \mathcal{X} \rightarrow \mathbb{R}$ denotes an information measure that typically would depend on $F_{\Theta, k}$, and $m_k$ corresponds to the number of queries desired at round $k$. However, for $m_k > 1$, this selection strategy can lead to a redundant query set as each query therein is selected independently of the others. The sub-field of batch AL is concerned with this issue and developing strategies to ensure some notion of diversity in the query set [5, 22, 28]. For instance, BatchBALD [29] relies on minimising the mutual information between pairs of queries in $Q_k$.

Table 2: Open source libraries for AL and features available. (*) ModAL can work with models defined in Keras and PyTorch via additional libraries such as Skorch [30] which provides them with an interface akin to Scikit-learn estimators. (†) Scikit-activeml lists a future update for regression strategies as does ALiPY. (‡) Google’s AL playground has utilities for defining a dataset compatible with the sample strategies, as well as sample datasets to test this utility, but no verification on whether these datasets have been used for active learning in literature nor utilities for setting up AL task configurations.

| Name (Year)          | Main ML framework | Additional ML frameworks officially supported | Strategies | Strategies Classification | Strategies Regression | Bayesian approximation | Explicit data managing | Datasets | Licence     |
|----------------------|-------------------|---------------------------------------------|------------|---------------------------|----------------------|------------------------|------------------------|----------|-------------|
| Google Active Learning (2019) | Keras/TF          | None                                        | Yes        | No                        | No                   | No                     | Yes†                   | Yes| Apache 2.0 |
| JCLAL [31] (2016)    | Weka/MULAN        | None                                        | Yes        | No                        | No                   | Yes                    | No                     |        | GPL 3.0     |
| scikit-activeml [22] (2021) | Scikit-learn      | None                                        | Yes        | No                        | No                   | No                     | Yes                    | No| BSD-3-Clause |
| AlPy [33] (2019)     | Generic           | NA                                          | Yes        | No                        | No                   | Yes                    | No                     | No| BSD-3-Clause |
| LibCtF [34] (2017)   | Scikit-learn      | None                                        | Yes        | No                        | No                   | Yes                    | No                     |        | BSD-2-Clause |
| CardinAL [35] (2022) | Scikit-learn      | None                                        | Yes        | No                        | No                   | No                     | No                     |        | Apache 2.0 |
| BAAL [66] (2020)     | PyTorch           | Scikit-learn                                | Yes        | Yes                       | Yes                  | Yes                    | No                     | No| Apache 2.0 |
| ModAL [37] (2018)    | Scikit-learn      | Keras/PyTorch*                              | Yes        | Yes                       | Yes                  | Yes                    | No                     | No| MIT         |
| PyRelationAL [38]    | Generic/PyTorch   | Scikit-learn/TF/Keras/fax                   | Yes        | Yes                       | Yes                  | Yes                    | Yes                    | No| Apache 2.0 |

3 Design principles and positioning within the ML and AL infrastructure ecosystem

AL pipelines can appear under various scenarios such as pool-, streaming-, or membership query-based sampling. All three involve complex interactions with the underlying labelled training data, the learning algorithm, and the AL strategies. Similarly AL strategies can evolve from simple sequential uncertainty sampling approaches to complex agents that leverage several informative measures and query selection algorithms in conjunction [5, 23].

PyRelationAL was developed under careful consideration of features available within the existing AL ecosystem, coupled with our vision to create a researcher-first imperative style library for AL research and development. To accommodate the growing complexity, advancements in new ML infrastructures and encourage user construction of complex AL pipelines and strategies, we strove to make writing of data managers, ML models, and AL strategies as intuitive and productive as possible. This is achieved through a modular framework which we describe in Section 4. To encourage the immediate use, study, and extension of existing strategies we have implemented various informativeness measures and query strategies that can be composed arbitrarily to re-implement or devise novel AL methods in classification and regression tasks in our tutorials and examples. Furthermore, in recognition of increasing use of deep learning models within AL pipelines, we provide modules that allow approximate Bayesian inference with point estimate models such as MCDropout [27].

There are a number of open source libraries dedicated to AL whose features are summarised in Table 2. As the table shows, most libraries are tied to a particular ML framework with specific strategies
revolving around the available ML model types, all with differing levels of coverage both across classification and regression tasks. Each library comes with different goals in mind and they should be appreciated for addressing different needs in open source research. ModAL [37] is an excellent modular python library for AL built with Scikit-learn as a basis for models. Its design emphasis on modularity and extensibility makes it the most similar to our work. Yet we differ to this and other libraries by making the user explicitly care about the dataset and how the model, strategy and oracle can interact with it through a data manager (see Section 4), controlling all aspects of AL pipeline as well as the function of the strategy. The flexible nature of our modules may be seen as a limitation that incurs additional development overhead compared to other libraries but we believe this trade-off is practical and useful to researchers exploring new approaches. As we outline in Section 5 another important contribution of our library is an API for downloading selected datasets and constructing AL benchmarks or tasks. As such we believe that PyRelationAL offers a compelling and complete set of features that is complementary and additive to the existing ML and the AL tools ecosystem. In the next section we describe how our modules enable quick development of AL with the practical flexibility to create novel pipelines and strategies.

4 PyRelationAL framework design

PyRelationAL decomposes the steps discussed in the Section 2 in three primary modules, as illustrated in Figure 1, a data manager, a ML manager, and an AL strategy. Figure 2 provides schematic of these modules using Universal Modelling Language (UML) diagrams to highlight the major attributes and methods of each module. Appendix B showcases a use case of PyRelationAL through a full coding example.

![Diagram of the three constitutive modules of PyRelationAL](image)

**Data manager** This module is designed to work with any PyTorch Dataset object, which in turn can be used flexibly with other numerical libraries through custom collate functions, as illustrated in PyRelationAL suite of examples. The job of the data manager is multi-faceted: it stores the dataset, keeps track of data subsets, handles the creation of dataloaders for each subset, and finally interacts with the oracle to update after each loop. Note that, the validation set and test set are considered external to the AL loop and can be used for model selection and evaluation purposes.

**ML manager** In our theoretical framing, this second major component defines $F_{\theta,k}$ from which uncertainties can be estimated and used as basis for query selection. In practice this module manages the life-cycle of the learning algorithm from instantiation to evaluation, through training and uncertainty estimation. While PyRelationAL natively offers multiple ML managers using PyTorch and PyTorch Lightning [38] as a training engine, we demonstrate through tutorials and examples that any ML framework can be interfaced with PyRelationAL using our ML manager interface.

**AL strategy** The crux of an AL iteration is the strategy which relies on a notion of informativeness $I$ and a selection criterion to define $Q_k$ at each iteration $k$ (see Figure 3 for pool-based AL). Note that in some AL strategies, the informativeness notion and the selection criterion are not separable.
Informativeness
Selection
AL strategy

Figure 3: Illustration of the flow of the active learning strategy during one iteration in the pool-based AL framing. The unlabelled set is fed to the active learning strategy which typically would first score each sample according to its notion of informativeness before selecting a query set based on its selection strategy given the samples and their scores.

Table 3: List of informativeness measures implemented in PyRelationAL currently. The task column indicates whether the corresponding informativeness measure is defined for classification, regression, or is agnostic (Any) to the ML task being performed.

| Name                     | Task              | Ref. |
|--------------------------|-------------------|------|
| Entropy                  | Classification    | [39, 5] |
| Least confidence         | Classification/Regression | [40, 5] |
| Margin confidence        | Classification    | [41, 5] |
| Ratio confidence         | Classification    | [41] |
| Greedy score             | Regression        | [42] |
| Upper confidence bound   | Regression        | [42] |
| Expected improvement     | Regression        | [42] |
| Bayesian active learning by disagreement | Classification/Regression | [43] |
| Thompson sampling        | Regression        | [44] |
| Representative sampling  | Any               | [45] |
| Relative distance        | Any               | [46] |

The informativeness measure is often task-dependent; for instance, uncertainty measures are computed differently for continuous and categorical targets. Table 3 gives the list of informativeness measures from the literature that are implemented in PyRelationAL and Appendix A provides more details and discussion around the various measures. Note that all individual informativeness measure can be combined together. For instance, the Upper Confidence Bound (UCB) score for regression as defined in [42] is a linear combination of the greedy score and least confidence score for regression tasks, with trade-off controlled by a hyperparameter. The final step is to select \( Q_k \) from \( U_k \) based on a chosen criteria combined with the informativeness scores.

5 Benchmark datasets and AL tasks

A core part of ML research and development is the translation of theory to practice typically in the form of evaluating a proposed method empirically against a range of established or challenging benchmark datasets and tasks. The practice of empirically evaluating on established datasets and tasks has become so ubiquitous that all major ML frameworks such as PyTorch, TensorFlow, SciKit-Learn come with interfaces for downloading common benchmarks. The rapid progress of ML research in images, text, and graphs can be attributed at least partially to easy access to pre-processed benchmark datasets [47, 48, 49, 50].

However, despite a multitude of papers, surveys, and other libraries for AL methods there is no established set of datasets evaluating AL strategies. To further complicate matters the same datasets can be processed to pose different AL tasks such as cold and warm starts as described in Konyushkova et al. [20] and Yang and Loog [21] to provide different challenges to strategies. In other words, a benchmark for AL has to be considered from the characteristics of the dataset and the circumstances of the initial labelling.

Due to these challenges, AL papers have a tendency to test and apply proposed methods using different splits of the same datasets with little overlap agreement across papers — as noted in several reviews [9, 21, 64]. This makes it difficult to assess strategies horizontally across a range of common
Table 4: Selection of datasets made available in the PyRelationAL library along with information on whether the ML task is a classification or regression, whether it is real-world or synthetic dataset, and the raw source of our implementation or the paper from which we constructed the dataset if it was not available publicly. We also give the licence of each dataset curated and extend our permissive Apache 2.0 licence (see section 6) to synthetic datasets generated with our code as well as the task configurations. Our selection was strongly based on their prior reference in related AL literature.

| Name           | ML Task  | Type   | Source | Use in AL literature | Licence   |
|----------------|----------|--------|--------|----------------------|-----------|
| CreditCard     | Classification | Real    | [51]   | [20]                 | DbCL 1.0  |
| StriatumMini   | Classification | Real    | [52, 53, 20] | [20, 54] | GPLv3     |
| Breast         | Classification | Real    | [55]   | [56, 21, 9]          | CC BY 4.0 |
| Glass          | Classification | Real    | [55]   | [57, 58, 9]          | CC BY 4.0 |
| Parkinsons     | Classification | Real    | [59, 55] | [60, 21, 9] | CC BY 4.0 |
| SynthClass1    | Classification | Synthetic | [21]  | [21]                 | Apache 2.0 |
| SynthClass2    | Classification | Synthetic | 61    | 61, 21               | Apache 2.0 |
| GaussianClouds | Classification | Synthetic | 20    | 20, 21               | Apache 2.0 |
| Checkerboard2x2| Classification | Synthetic | 20    | 20                   | Apache 2.0 |
| Checkerboard4x4| Classification | Synthetic | 20    | 20                   | Apache 2.0 |
| Diabetes       | Regression  | Real    | [62, 55] | [56, 9]              | CC BY 4.0 |
| Concrete       | Regression  | Real    | [63, 55] | 64                  | CC BY 4.0 |
| Energy         | Regression  | Real    | [65, 55] | 66                  | CC BY 4.0 |
| Power          | Regression  | Real    | [67, 55] | [66, 64]            | CC BY 4.0 |
| Airfoil        | Regression  | Real    | 55     | 64                  | CC BY 4.0 |
| WineQuality    | Regression  | Real    | [68, 55] | 64                  | CC BY 4.0 |
| Yacht          | Regression  | Real    | 55     | [66, 64]            | CC BY 4.0 |

datasets and identify regimes under which a given strategy shows success or failure. This issue is exacerbated by publication bias which favours the reporting of positive results — as noted in Settles [5]. To help alleviate this issue we have collected a variety of datasets for both classification and regression tasks as used in AL literature and make these available through PyRelationAL, see Table 4. The datasets are either real world datasets or synthetic datasets taken from seminal AL literature [20, 51, 9, 21, 64, 66]. The synthetic datasets were typically devised to pose challenges to specific strategies. Another selection criteria was their permissive licensing, such as the Creative Commons Attribution 4.0 International License granted on the recently updated UCI archives [55], or the licenses through the Open Data Commons initiative.

Each of the datasets can be downloaded and processed into PyTorch Dataset objects through a simple API. Furthermore, we provide additional facilities to turn them into PyRelationAL DataManager objects that emulate cold and warm start AL initialisations with arbitrary train-validation-test splits and canonical splits (where applicable) for pain-free benchmarking.

In Figure 4 we show the performance curves over query iterations using a Gaussian process classifier with 5 different budgeted AL strategies on the Checkerboard2x2 dataset from Konyushkova et al. [20]. Our intent with this example is first to show drastic economies that can be obtained with active learning in early stages of labelling (i.e. AL is useful!) and secondly how dramatically these curves may change based on the task configuration within a dataset. We show the importance of the initial AL task configurations within datasets and demonstrate that there is no free-lunch amongst the AL strategies. Such results motivate the collection of datasets and task configurations, as well our modular approach to constructing methods so that researchers can modify and study the behaviours of novel strategies quickly. We provide a more comprehensive comparative analysis across the currently available datasets in Table 4 with details on the experimental setup as used here in Appendix C.

6 Maintaining PyRelationAL

We consider AL as an important tool and a growing domain of research interest, particularly as ML research focus intensifies towards tasks in low-data regimes such as biomedicine. Hence, we adopt modern open source software engineering practices in order to promote robustness and reliability of
Figure 4: Performance curves over serial query iterations of selected active learning strategies on the Checkerboard2x2Dataset from Konyushkova et al. [20]. The left figure shows the balanced accuracy given a cold start task configuration, the right figure shows the performance given a warm start configuration.

(a) Cold start
(b) Warm start

7 Conclusion

PyRelationAL supports popular modelling frameworks and flexibly accounts for the various components within an AL pipeline. We provide detailed documentation and various tutorials across use cases. Furthermore, we adopt modern software practices with an inclusive code of conduct as discussed in Section 6 to foster a productive, sustainable and healthy growth of the library and the community around it. We endeavoured to release PyRelationAL as both a tool to help practitioners perform research but also help newcomers join the community and make novel contributions to the field. We therefore believe PyRelationAL offers a compelling set of features that are additive and beneficial to the AL community.
References

[1] Thomas Gaudelet, Ben Day, Arian R Jamash, Jyothish Soman, Cristian Regep, Gertrude Liu, Jeremy B R Hayter, Richard Vickers, Charles Roberts, Jian Tang, David Roblin, Tom L Blundell, Michael M Bronstein, and Jake P Taylor-King. Utilizing graph machine learning within drug discovery and development. *Briefings in Bioinformatics*, 22(6), 05 2021. bbab159.

[2] Justin S Smith, Ben Nebgen, Nicholas Lubbers, Olexandr Isayev, and Adrian E Roitberg. Less is more: Sampling chemical space with active learning. *The Journal of Chemical Physics*, 148(24):241733, 2018.

[3] Mohammed Abdelwahab and Carlos Busso. Active learning for speech emotion recognition using deep neural network. In *2019 8th International Conference on Affective Computing and Intelligent Interaction (ACII)*, pages 1–7. IEEE, 2019.

[4] Steven CH Hoi, Rong Jin, Jianke Zhu, and Michael R Lyu. Batch mode active learning and its application to medical image classification. In *Proceedings of the 23rd International Conference on Machine Learning*, pages 417–424, 2006.

[5] Burr Settles. Uncertainty sampling. In *Active Learning*, Synthesis Lectures on Artificial Intelligence and Machine Learning, pages 11–21. Morgan & Claypool Publishers, 2012.

[6] Eric Brochu, Vlad M Cora, and Nando De Freitas. A tutorial on bayesian optimization of expensive cost functions, with application to active user modeling and hierarchical reinforcement learning. *arXiv preprint arXiv:1012.2599*, 2010.

[7] Richard S Sutton and Andrew G Barto. *Reinforcement learning: An introduction*. MIT press, 2018.

[8] Pengzhen Ren, Yun Xiao, Xiaojun Chang, Po-Yao Huang, Zhihui Li, Brij B Gupta, Xiaojiang Chen, and Xin Wang. A survey of deep active learning. *ACM Computing Surveys (CSUR)*, 54(9):1–40, 2021.

[9] Xueying Zhan, Huan Liu, Qing Li, and Antoni B. Chan. A comparative survey: Benchmarking for pool-based active learning. In Zhi-Hua Zhou, editor, *Proceedings of the Thirtieth International Joint Conference on Artificial Intelligence, IJCAI-21*, pages 4679–4686. International Joint Conferences on Artificial Intelligence Organization, 8 2021. Survey Track.

[10] Brian Hie, Bryan D Bryson, and Bonnie Berger. Leveraging uncertainty in machine learning accelerates biological discovery and design. *Cell Systems*, 11(5):461–477, 2020.

[11] Paul Bertin, Jarrid Rector-Brooks, Deepak Sharma, Thomas Gaudelet, Andrew Anighoro, Torsten Gross, Francisco Martinez-Pena, Eileen L Tang, Cristian Regep, Jeremy Hayter, et al. Recover: sequential model optimization platform for combination drug repurposing identifies novel synergistic compounds in vitro. *arXiv preprint arXiv:2202.04202*, 2022.

[12] Arash Mehrjou, Ashkan Soleymani, Andrew Jesson, Pascal Notin, Yarin Gal, Stefan Bauer, and Patrick Schwab. GeneDisco: A Benchmark for Experimental Design in Drug Discovery. *arXiv:2110.11875 [cs, stat]*, October 2021. arXiv: 2110.11875.

[13] Adam Paszke, Sam Gross, Francisco Massa, et al. Pytorch: An imperative style, high-performance deep learning library. In H. Wallach, H. Larochelle, A. Beygelzimer, F. d’Alché-Buc, E. Fox, and R. Garnett, editors, *Advances in Neural Information Processing Systems 32*, pages 8024–8035. Curran Associates, Inc., 2019.

[14] François Chollet et al. Keras. [*https://keras.io*](https://keras.io) 2015.

[15] James Bradbury, Roy Frostig, Peter Hawkins, Matthew James Johnson, Chris Leary, Dougal Maclaurin, George Necula, Adam Paszke, Jake VanderPlas, Skye Wanderman-Milne, and Qiao Zhang. JAX: composable transformations of Python+NumPy programs, 2018.

[16] Jonathan Heek, Anselm Levskaya, Avital Oliver, Marvin Ritter, Bertrand Rondepierre, Andreas Steiner, and Marc van Zee. Flax: A neural network library and ecosystem for JAX, 2020.

[17] Dustin Tran, Matthew D. Hoffman, Rif A. Saurous, Eugene Brevdo, Kevin Murphy, and David M. Blei. Deep probabilistic programming. In *International Conference on Learning Representations*, 2017.

[18] Jacob R Gardner, Geoff Pleiss, David Bindel, Kilian Q Weinberger, and Andrew Gordon Wilson. Gpytorch: Blackbox matrix-matrix gaussian process inference with gpu acceleration. In *Advances in Neural Information Processing Systems*, 2018.
[19] Du Phan, Neeraj Pradhan, and Martin Jankowiak. Composable effects for flexible and accelerated probabilistic programming in numpyro. arXiv preprint arXiv:1912.11554, 2019.

[20] Ksenia Konyushkova, Raphael Sznitman, and Pascal Fua. Learning active learning from data. Advances in Neural Information Processing Systems, 30, 2017.

[21] Yazhou Yang and Marco Loog. A benchmark and comparison of active learning for logistic regression. Pattern Recognition, 83:401–415, 2018.

[22] Klaus Brinker. Incorporating diversity in active learning with support vector machines. In Proceedings of the Twentieth International Conference on International Conference on Machine Learning, ICML’03, page 59–66. AAAI Press, 2003.

[23] Robert (Munro) Monarch. Human-In-the-Loop Machine Learning: Active Learning and Annotation for Human-Centered AI. Manning Publications Co. LLC, 2021.

[24] Balaji Lakshminarayanan, Alexander Pritzel, and Charles Blundell. Simple and Scalable Predictive Uncertainty Estimation using Deep Ensembles. arXiv:1612.01474 [cs, stat], November 2017. arXiv: 1612.01474.

[25] David Cohn, Les Atlas, and Richard Ladner. Improving generalization with active learning. Machine Learning, 15(2):201–221, May 1994.

[26] H. S. Seung, M. Opper, and H. Sompolinsky. Query by committee. In Proceedings of the Fifth Annual Workshop on Computational Learning Theory, COLT ’92, page 287–294, New York, NY, USA, 1992. Association for Computing Machinery.

[27] Yarin Gal and Zoubin Ghahramani. Dropout as a bayesian approximation: Representing model uncertainty in deep learning. In International Conference on Machine Learning, pages 1050–1059. PMLR, 2016.

[28] Yuhong Guo and Dale Schuurmans. Discriminative batch mode active learning. In Proceedings of the 20th International Conference on Neural Information Processing Systems, NIPS’07, page 593–600, Red Hook, NY, USA, 2007. Curran Associates Inc.

[29] Andreas Kirsch, Joost Van Amersfoort, and Yarin Gal. Batchbald: Efficient and diverse batch acquisition for deep bayesian active learning. Advances in Neural Information Processing Systems, 32, 2019.

[30] Marian Tietz, Thomas J. Fan, Daniel Nouri, Benjamin Bossan, and skorch Developers. skorch: A scikit-learn compatible neural network library that wraps PyTorch, July 2017.

[31] Oscar Reyes, Eduardo Pérez, María del Carmen Rodríguez-Hernández, Habib M. Fardoun, and Sebastián Ventura. Jclal: A java framework for active learning. Journal of Machine Learning Research, 17(95):1–5, 2016.

[32] Daniel Kottke, Marek Herde, Tuan Pham Minh, Alexander Benz, Pascal Mergerd, Atal Rognman, Christoph Sandrock, and Bernhard Sick. scikitactiveml: A library and toolbox for active learning algorithms. Preprints, 2021.

[33] Ying-Peng Tang, Guo-Xiang Li, and Sheng-Jun Huang. ALiPy: Active learning in python. Technical report, Nanjing University of Aeronautics and Astronautics, January 2019. available as arXiv preprint https://arxiv.org/abs/1901.03802

[34] Yao-Yuan Yang, Shao-Chuan Lee, Yu-An Chung, Tung-En Wu, Si-An Chen, and Hsuan-Tien Lin. libact: Pool-based active learning in python. Technical report, National Taiwan University, October 2017. available as arXiv preprint https://arxiv.org/abs/1710.00379.

[35] Alexandre Abraham and Léo Dreyfus-Schmidt. Cardinal, a metric-based active learning framework. Software Impacts, 12:100250, 2022.

[36] Parmida Atighehchian, Frédéric Branchaud-Charron, and Alexandre Lacoste. Bayesian active learning for production, a systematic study and a reusable library. CoRR, abs/2006.09916, 2020.

[37] Tivadar Danka and Peter Horvath. modal: A modular active learning framework for python. arXiv preprint arXiv:1805.00979, 2018.

[38] William Falcon, Jirka Borovec, Adrian Wäldli, et al. Pytorchlightning/pytorch-lightning: 0.7.6 release, May 2020.
[39] Ido Dagan and Sean P. Engelson. Committee-based sampling for training probabilistic classifiers. In Proceedings of the Twelfth International Conference on International Conference on Machine Learning, ICML’95, page 150–157, San Francisco, CA, USA, 1995. Morgan Kaufmann Publishers Inc.

[40] David D. Lewis and Jason Catlett. Heterogeneous uncertainty sampling for supervised learning. In William W. Cohen and Haym Hirsh, editors, Machine Learning Proceedings 1994, pages 148–156. Morgan Kaufmann, San Francisco (CA), 1994.

[41] Tobias Scheffer, Christian Decomain, and Stefan Wrobel. Active hidden markov models for information extraction. In Proceedings of the 4th International Conference on Advances in Intelligent Data Analysis, IDA ’01, page 309–318, Berlin, Heidelberg, 2001. Springer-Verlag.

[42] George De Ath, Richard M Everson, Alma AM Rahat, and Jonathan E Fieldsend. Greed is good: Exploration and exploitation trade-offs in bayesian optimisation. ACM Transactions on Evolutionary Learning and Optimization, 1(1):1–22, 2021.

[43] Neil Houlsby, Ferenc Huszár, Zoubin Ghahramani, and Máthé Lengyel. Bayesian active learning for classification and preference learning. arXiv preprint arXiv:1112.5745, 2011.

[44] Daniel J Russo, Benjamin Van Roy, Abbas Kazerouni, Ian Osband, Zheng Wen, et al. A tutorial on Thompson sampling. Foundations and Trends in Machine Learning, 11(1):1–96, 2018.

[45] Hieu T. Nguyen and Arnold Smeluders. Active learning using pre-clustering. In Proceedings of the Twenty-First International Conference on Machine Learning, ICML ’04, page 79, New York, NY, USA, 2004. Association for Computing Machinery.

[46] Sanjoy Dasgupta and Daniel Hsu. Hierarchical sampling for active learning. In Proceedings of the 25th International Conference on Machine Learning, ICML ’08, page 208–215, New York, NY, USA, 2008. Association for Computing Machinery.

[47] J. Deng, W. Dong, R. Socher, L.-J. Li, K. Li, and L. Fei-Fei. ImageNet: A Large-Scale Hierarchical Image Database. In Computer Vision and Pattern Recognition, 2009.

[48] Alex Wang, Yada Pruksachatkun, Nikita Nangia, Amanpreet Singh, Julian Michael, Felix Hill, Omer Levy, and Samuel Bowman. Superglue: A stickier benchmark for general-purpose language understanding systems. Advances in Neural Information Processing Systems, 32, 2019.

[49] Weihua Hu, Matthias Fey, Marinka Zitnik, Yuxiao Dong, Hongyu Ren, Bowen Liu, Michele Catusta, and Jure Leskovec. Open graph benchmark: Datasets for machine learning on graphs. Advances in Neural Information Processing Systems, 33:22118–22133, 2020.

[50] Kexin Huang, Tianfan Fu, Wenhao Gao, Yue Zhao, Yusuf Roohani, Jure Leskovec, Connor W Coley, Cao Xiao, Jimeng Sun, and Marinka Zitnik. Therapeutics dat commons: Machine learning datasets and tasks for drug discovery and development. arXiv preprint arXiv:2102.09548, 2021.

[51] Andrea Dal Pozzolo, Olivier Caelen, Reid A. Johnson, and Gianluca Bontempi. Calibrating probability with undersampling for unbalanced classification. In 2015 IEEE Symposium Series on Computational Intelligence, pages 159–166, 2015.

[52] Aurélien Lucchi, Yunpeng Li, and Pascal Fua. Learning for structured prediction using approximate subgradient descent with working sets. In 2013 IEEE Conference on Computer Vision and Pattern Recognition, pages 1987–1994, 2013.

[53] Aurélien Lucchi, Yunpeng Li, Kevin Smith, and Pascal Fua. Structured image segmentation using kernelized features. In European conference on computer vision, pages 400–413. Springer, 2012.

[54] Ksenia Konyushkova, Raphael Sznitman, and Pascal V. Fua. Introducing geometry in active learning for image segmentation. 2015 IEEE International Conference on Computer Vision (ICCV), pages 2974–2982, 2015.

[55] Dheeru Dua and Casey Graff. UCI machine learning repository, 2017.

[56] Neil Houlsby, Ferenc Huszár, Zoubin Ghahramani, and Máthé Lengyel. Bayesian active learning for classification and preference learning. arXiv preprint arXiv:1112.5745, 2011.

[57] Wenbin Cai, Ya Zhang, and Jun Zhou. Maximizing expected model change for active learning in regression. In 2013 IEEE 13th International Conference on Data Mining, pages 51–60, 2013.
[58] Bo Du, Zengmao Wang, Lefei Zhang, Liangpei Zhang, Wei Liu, Jialie Shen, and Dacheng Tao. Exploring representativeness and informativeness for active learning. *IEEE Transactions on Cybernetics*, 47(1):14–26, 2017.

[59] Max A. Little, Patrick E. McSharry, Stephen J. Roberts, Declan AE Costello, and Irene M. Moroz. Exploiting nonlinear recurrence and fractal scaling properties for voice disorder detection. *BioMedical Engineering OnLine*, 6(1):23, Jun 2007.

[60] Sicheng Xiong, Javad Azimi, and Xiaoli Z. Fern. Active learning of constraints for semi-supervised clustering. *IEEE Transactions on Knowledge and Data Engineering*, 26(1):43–54, 2014.

[61] Sheng-Jun Huang, Songcan Chen, and Zhi-Hua Zhou. Multi-label active learning: Query type matters. In *Proceedings of the 24th International Conference on Artificial Intelligence*, IJCAI'15, page 946–952. AAAI Press, 2015.

[62] Bradley Efron, Trevor Hastie, Iain Johnstone, and Robert Tibshirani. Least angle regression. *The Annals of Statistics*, 32(2):407 – 499, 2004.

[63] L.-C. Yeh. Modeling of strength of high-performance concrete using artificial neural networks. *Cement and Concrete Research*, 28(12):1797–1808, 1998.

[64] Dongrui Wu. Pool-based sequential active learning for regression. *IEEE Transactions on Neural Networks and Learning Systems*, 30(5):1348–1359, 2019.

[65] Athanasios Tsanas and Angeliki Xifara. Accurate quantitative estimation of energy performance of residential buildings using statistical machine learning tools. *Energy and Buildings*, 49:560–567, 2012.

[66] Robert Pinsler, Jonathan Gordon, Eric Nalisnick, and José Miguel Hernández-Lobato. Bayesian batch active learning as sparse subset approximation. *Advances in Neural Information Processing Systems*, 32, 2019.

[67] Pınar Tüfekci. Prediction of full load electrical power output of a base load operated combined cycle power plant using machine learning methods. *International Journal of Electrical Power & Energy Systems*, 60:126–140, 2014.

[68] Paulo Cortez, António Cerdeira, Fernando Almeida, Telmo Matos, and José Reis. Modeling wine preferences by data mining from physicochemical properties. *Decision Support Systems*, 47(4):547–553, 2009. Smart Business Networks: Concepts and Empirical Evidence.

[69] Armen Der Kiureghian and Ove Ditlevsen. Aleatory or epistemic? does it matter? *Structural Safety*, 31(2):105–112, 2009.

[70] Claude Elwood Shannon. A mathematical theory of communication. *The Bell System Technical Journal*, 27:379–423, 1948.

[71] F. Pedregosa, G. Varoquaux, A. Gramfort, V. Michel, B. Thirion, O. Grisel, M. Blondel, P. Prettenhofer, R. Weiss, V. Dubourg, J. Vanderplas, A. Passos, D. Cournapeau, M. Brucher, M. Perrot, and E. Duchesnay. Scikit-learn: Machine learning in Python. *Journal of Machine Learning Research*, 12:2825–2830, 2011.

[72] Carl Edward Rasmussen and Christopher K. I. Williams. *Gaussian processes for machine learning*, volume 2. MIT Press, 2006.

[73] Yaniv Ovadia, Emily Fertig, Jie Ren, Zachary Nado, David Sculley, Sebastian Nowozin, Joshua Dillon, Balaji Lakshminarayanan, and Jasper Snoek. Can you trust your model’s uncertainty? evaluating predictive uncertainty under dataset shift. *Advances in Neural Information Processing Systems*, 32, 2019.

[74] Dan Hendycks and Kevin Gimpel. A baseline for detecting misclassified and out-of-distribution examples in neural networks. *arXiv preprint arXiv:1610.02136*, 2016.

[75] Zoubin Ghahramani. Probabilistic machine learning and artificial intelligence. *Nature*, 521(7553):452–459, 2015.

[76] Wesley J. Maddox, Timur Garipov, Pavel Izmailov, Dmitry Vetrov, and Andrew Gordon Wilson. *A Simple Baseline for Bayesian Uncertainty in Deep Learning*. Curran Associates Inc., Red Hook, NY, USA, 2019.
A Informativeness measures

In this section, we provide more details about each type of informativeness measure discussed in the main and described some of the specific scores mentioned in Table 3.

A.1 Uncertainty-based informativeness scores

As discussed in Section 4, a large number of informativeness measures rely on some estimate of prediction uncertainties. The underlying rationale is that regions of the world are highly uncertain because they are poorly represented in the training data. Improving coverage through sampling uncertain data regions can enable significant global performance gains. While this makes intuitive sense, it ignores subtleties about the nature of uncertainties which can be decomposed in epistemic and aleatoric components [69]. The former is understood as coming from modelling errors while the latter is inherent to the world, corresponding to natural variations or measurement noise. Aleatoric uncertainties are irreducible and, in practice, it is extremely difficult to tease out the two uncertainty components from each other. This means that uncertainty-based informativeness scores can overestimate the information gain that a sample would provide.

In the following, we detail a few of the scores that fall under this category.

**Entropy** is a well-established notion in information theory that quantifies the uncertainty of a probability distribution over possible outcomes [70]. It is used as an informativeness measure for classification tasks where the probability distribution is defined over the finite set of labels $Y$. Specifically, it is defined as

$$I(x) = - \sum_{y \in Y} p_{F_{\theta,k}}(y|x) \log(p_{F_{\theta,k}}(y|x)).$$

**Least confidence** can be used both for regression and classification tasks, although the score is defined differently for each task. In regression tasks, we have

$$I(x) = \text{Var}_{F_{\theta,k}}[Y|x],$$

where $Y$ denotes a random variable in $Y$. Hence, to each sample $x$ it associates the variance across the predictions from the set of functions $F_{\theta,k}$.

In classification tasks, the least confidence score is defined as

$$I(x) = 1 - \max_{y \in Y} p_{F_{\theta,k}}(y|x).$$

**Margin confidence** was introduced for classification tasks and measures uncertainty as the difference between the highest and second highest probabilities associated to labels in $Y$ derived from our predictions on a given sample. The smaller that difference, the higher the uncertainty. In equation, this gives

$$y_0 = \arg\max_{y \in Y} p_{F_{\theta,k}}(y|x),$$

$$y_1 = \arg\max_{y \in Y \setminus \{y_0\}} p_{F_{\theta,k}}(y|x),$$

$$I(x) = 1 - \left(p_{F_{\theta,k}}(y_0|x) - p_{F_{\theta,k}}(y_1|x)\right).$$

**Ratio confidence** is a score similar to margin confidence, the only difference comes from the fact that the uncertainty is expressed as a ratio between the two probabilities

$$y_0 = \arg\max_{y \in Y} p_{F_{\theta,k}}(y|x),$$

$$y_1 = \arg\max_{y \in Y \setminus \{y_0\}} p_{F_{\theta,k}}(y|x),$$

$$I(x) = \frac{p_{F_{\theta,k}}(y_1|x)}{p_{F_{\theta,k}}(y_0|x)}.$$
**Greedy score**  This is a simple score used for regression tasks where greater values in $\mathcal{Y}$ are of higher interest. For instance, we would be more interested in reliably identifying highly synergistic pairs of drugs. The score is defined as

$$I(x) = \mathbb{E}_{\mathcal{F}_{\theta,k}} [Y|x].$$

**Upper confidence bound**  UCB comes from the reinforcement learning (RL) literature and corresponds to a trade-off, controlled by an hyperparameter $\lambda$, between the greedy score and the least confidence score. It is formally defined as

$$I(x) = \mathbb{E}_{\mathcal{F}_{\theta,k}} [Y|x] + \lambda \sqrt{\text{Var}_{\mathcal{F}_{\theta,k}} [Y|x]},$$

where $Y$ denotes a random variable in $\mathcal{Y}$.

Similarly to the greedy score, it is defined for continuous label values and assumes that greater values, known as rewards in RL, are more relevant to the problem.

**A.2 Diversity-based informativeness scores**

Rather than rely on some estimate of uncertainties, diversity-based scores aim to increase the diversity of the training set, querying samples that are far from the current labelled set according to a selected distance metric. Methods can differ on the choice of distance metric and on the space where distances are computed. The ambient space is often used but can have some limitations due to noisy or redundant features or suffer from the curse of dimensionality in high-dimensional space. As such, researchers have proposed to compute distances in lower dimensional spaces either obtained from dimensionality reduction techniques or from intermediary latent spaces derived from a trained model. We discuss below two generic types of approaches that are built-in PyRelationAL.

**Relative distance sampling**  computes the minimum distance from an unlabelled sample to the labelled samples

$$I(x) = \min_{l \in L} d \left( \phi(x), \phi(l) \right),$$

where $\phi : \mathcal{X} \mapsto \mathbb{R}^m$ an embedding function projecting samples into a latent space and $d : \mathbb{R}^m \times \mathbb{R}^m \mapsto \mathbb{R}_+$ represents the chosen distance metric in the latent space. Note that $\phi$ is simply the identity function when computing distances in the ambient space. The coreset approach, as defined in [12], would be classified in this category in PyRelationAL, where the latent space representation of a point is defined by the associated penultimate activations in a neural network.

**Representative sampling**  does not explicitly define an informativeness scores. Instead, it groups the current unlabelled set into a fixed number of clusters and selects representative samples from each cluster to form the query set. Note that this can be quite expensive to compute when the unlabelled set is large as it requires all-to-all pairwise distances, and can benefit from extracting first a subset of the unlabelled set based on some other criteria.

**B  Use case study: coding example**

In this section, we will walk through a simple coding example to showcase PyRelationAL building blocks and how to simply create an AL pipeline with them.

First, we need to define our dataset of interest, defined in Listings[1]. For this example we outline how one can outline their own custom datasets. We use the diabetes dataset from Scikit-Learn [71] package which contains data for 442 patients, each described by 10 features (such as age, sex, and bmi) and associated with a scalar score quantifying the disease’s progression, or stage. The distribution of these scores is shown in Figure[5].

```python
1 import torch
2 from sklearn.datasets import load_diabetes
3 from torch.utils.data import Dataset
4
5```
class DiabetesDataset(Dataset):
    def __init__(self):
        # Load the diabetes dataset
        diabetes_X, diabetes_y = load_diabetes(
            return_X_y=True
        )
        self.x = torch.FloatTensor(diabetes_X)
        self.y = torch.FloatTensor(diabetes_y)
    def __len__(self):
        return self.x.shape[0]
    def __getitem__(self, idx):
        return self.x[idx], self.y[idx]

Listing 1: Creating a pytorch dataset for a regression task using the Diabetes dataset from scikit-learn.

We then wrap the dataset into a PyRelationAL data manager (see Listings [2]), randomly splitting the data into train, validation, and test sets (lines 9-16) and taking a portion of the train set as our initial labelled set (lines 17-21).

def get_data_manager(
    batch_size=10,
    hit_ratio_at=5,
):
    ds = DiabetesDataset()
    train_ds, valid_ds, test_ds = \
    torch.utils.data.random_split(
        ds,
        [400, 22, 20],
    )
    train_indices = train_ds.indices
    valid_indices = valid_ds.indices
    test_indices = test_ds.indices
    labelled_indices = {
        train_indices[:labelled_size

Figure 5: Distribution of the diabetes progression score in the dataset considered.
Listing 2: Defining a PyRelationAL data manager for the dataset.

Second, we define a simple multi-layer perceptron model (see Listings 3) to predict diabetes progression based on the input features describing each patient.

Listing 3: A simple MLP regression pytorch model.

We then define a PyRelationAL ML manager to wrap around the PyTorch model in Listings 4, overriding the methods train (lines 20-36) and test (lines 38-48). We’ll use ensembling as a way to estimate prediction uncertainties, hence we use PyRelationAL’s GenericEnsembleModel as a base class. The base class handles instantiation of an ensemble of models of size governed by the n_estimators parameter (line 11).
Listing 4: Defining a torch model wrapper for PyRelationAL.

The last piece is the AL strategy. Here, we implement an ϵ-greedy strategy (see Listings[5]), borrowed from the reinforcement learning literature, that interpolates between a random strategy, that selects patients for labelling at random, and a greedy strategy, that selects patients whose diabetes is predicted to be most advanced, and who might be in need of more care.
scores = regression_greedy_score(x=output)
ixs = torch.argsort(
    scores, descending=True
).tolist()
greedy_annotate = int((1-self.eps)*num_annotate)
ixs = [self.u_indices[i] \\
    for i in ixs[: greedy_annotate]]
remaining_u_indices = list(
    set(self.u_indices) - set(ixs)
)
random_annotate = np.random.choice(  
    remaining_u_indices,
    num_annotate-greedy_annotate,
    replace=False,
)
return ixs + random_annotate.tolist()

Listing 5: Implements an $\epsilon$-greedy strategy, whereby a percentage of the samples to annotate are selected randomly while the remaining are selected greedily.

We now have everything ready to setup and run the AL pipeline (see Listings 6). Line 1 of the snippet defines a PyRelationAL data manager, line 2 create the PyRelationAL model. Both are then used to instantiate the strategy on line 8. On line 13, we estimate maximum theoretical performances that would be achieved if all the train set was available. Line 14 then performs an iterative AL loop whereby 25 patients from the unlabelled pool are added to the labelled set at each iteration.

data_manager = get_data_manager()
model = TorchModuleWrapper(
    DiabetesRegression,
    {"dropout": 0.12},
    {"epochs":100, "lr":3e-4},
    n_estimators=10,
)
strategy = EpsilonGreedyStrategy(
    data_manager=data_manager,
    model=model,
    eps=0.05
)
strategy.full_active_learning_run(num_annotate=25)

Listing 6: Running the strategy.

C Comparative analysis on selected strategies and datasets in PyRelationAL

In this section we perform a simple empirical comparative analysis of selected serial active learning strategies constructed with the informativeness measures in Table 3 across the current datasets in PyRelationAL. Serial active learning strategies perform one instance queries at each query loop iteration such that

$$Q_k = \arg \max_{q \in U_k} I(q),$$

and the strategy is mainly driven by the choice of informativeness measure $I(\cdot)$. We remind that our aim here is to show the different components at play when creating AL experiments and assessing the resulting performances of strategies rather than advocating for any method.

Inspired by Konyushkova et al. [20] and Yang and Loog [21], we assess our strategies on each dataset in two AL task configurations with respect to the ML task type.

- **Cold-start classification**: 1 observation for each class represented in the training set is labelled and the rest unlabelled.
• **Warm-start classification:** a randomly sampled 10 percent of the training set is labelled, the rest is unlabelled.

• **Cold-start regression:** the two observations with highest euclidean pairwise distance in the train set are labelled, the rest is unlabelled.

• **Warm-start regression:** a randomly sampled 10 percent of the training set is labelled, the rest is unlabelled.

**Experimental setup**  For each dataset, we use a 5-fold cross-validation setup (stratified for classification task). We generate a warm and cold start initialisation for each of these splits to set up an AL experiment. A single observation is queried at the end of each AL iteration, i.e. referred to the oracle for labelling. For small datasets (<300 observations in the training split) we run the query loop until all available observations in the training set are labelled. For larger datasets we set a maximum query budget of 250 iterations.

For the sake of simplicity, we used the same Gaussian process classifier (GPC) for each of the experiments on classification datasets and the same Gaussian process regressor (GPR) for the regression datasets. Both GPC and GPR utilise a RBF kernel. The model is trained anew at each AL query iteration. For both models, the prior is assumed to be constant and zero. The parameters of the kernel are optimized by maximizing the log marginal likelihood with the LBGFS algorithm. Details of the GPR implementation can be found in Algorithm 2.1 of Rasmussen and Williams [72]. The GPC implements the logistic link function based on Laplace approximation. Details of its implementation can be found in Algorithms 3.1, 3.2, and 5.1 of Rasmussen and Williams [72].

At each query iteration, we record the model’s balanced accuracy score for classification datasets and mean square error (MSE) for regression datasets on the respective hold-out test sets. We aggregate the performance curves over the AL iterations showing the mean performance and 95% confidence intervals over the data splits as displayed in Figures 6 and 7. We also aggregate the area under each AL iteration performance curve (shortened to IPAUC), this is a single number where higher numbers denote better performance of the strategy in classification and lower numbers are better in regression. We report the mean IPAUC score and standard deviations over all the curves. Obviously, different metrics can be used for the "performance" in the IPAUC score.

**Active learning strategies**  To keep the performance curves from being too cluttered in this paper, we report the performance on a chosen few strategies. For classification tasks, we use the 1) random acquisition, 2) least confidence, 3) margin confidence, 4) entropy, and 5) representative sampling strategies. For regression tasks, we use the 1) random acquisition, 2) least confidence, 3) BALD, 4) expected improvement, and 5) representative sampling strategies. These represent a small sample of methods coming from different families of AL approaches based on uncertainty sampling and diversity sampling techniques [5, 23].

All experiments were run on a single workstation with an Intel® Xeon® E5-1650 v3 CPU clocked at 3.50GHz and 64GB memory. All experimental scripts for replicating the experiments can be found in the supplementary materials alongside the library code base.

**Results and discussion**  First and foremost, as can be seen in the AL performance curves of Figures 6 and 7, considerable performance gains can be made economically via AL. We can see comparable results for models with far less annotated observations than those using the full dataset. The gains are especially obvious in cold start settings as shown by the results obtained for the Glass dataset in Figure 6c. However, we can also see that certain strategies bring benefits later on such as the BALD strategy in warm start Airfoil dataset (Figure 7b). As Tables 5 through 8 show, in equally many cases AL does not bring any tangible benefits compared to the baseline of randomly acquiring labels for samples.

Assessment of the active learning strategies requires consideration of several factors acting in conjunction: the dataset, the model class used, the way under which uncertainty is measured from the model (if relevant for the informativeness measure), and obviously the strategy itself. Below we discuss some of these considerations with reference to the results across Tables 5 to 8 and Figures 6 and 7.

The dataset and associated ML task have an effect on the AL performance through the model as a task may be too simple to solve for a model — as is evident by the saturated and largely
The choice of model affects strategies that utilise its notion of uncertainty to form informativeness measures. For example, the Gaussian process estimators we have utilised for the experiments provide principled measures of uncertainty. Meanwhile, a neural network can output class probabilities which can then be used to derive uncertainty estimates for informativeness measures. However, this is generally considered a poor uncertainty measure. Neural networks tend to produce pathologically overconfident predictions and struggle to quantify their uncertainty when applied on corrupted or previously unseen data [73, 74]. Bayesian modelling [75] as we have done with the GPs provides a theoretically rigorous approach to perform probabilistic inference also for deep neural networks. Seemingly these Bayesian neural networks (BNNs) combine the best of both worlds - the modelling complexity of a deep model augmented with uncertainty estimates through probabilistic inference over the weights of the neural network. Unfortunately the high computational cost of performing proper Bayesian inference restricts our use to using approximations. Many approximate Bayesian inference methods exist — such as MCDropout [27] and SWAG [76] — and each bring their own strengths, limitations, and hyperparameters that one can consider when assessing their downstream effects on AL strategies. Strategies designed to operate on committees and ensembles of models such as query-by-disagreement and query-by-committee algorithms work on similar principles and the collective of models gives rise informativeness measures whose quality and characteristics are dependent on its members.

As outlined in section 4, AL strategies can be defined through compositions of informativeness measures and query selection algorithms. Ultimately, the choice of strategy should be aligned with the objective of the practitioner. One objective of the active learning strategy can be to exploit model uncertainty to reduce classification error. This is useful for fine-tuning a model’s classification boundary and here uncertainty sampling techniques — such as the least confidence, margin, and entropy — succeed when ample representative data points are available as in the warm start configuration of Checkerboard2x2 in Figure 4b. Conversely, if the objective is to initially explore the input feature space, the serial uncertainty sampling strategies we have created can struggle immensely compared to random sampling baseline in Checkerboard2x2 cold start configuration in Figure 4a. This occurs as the myopic uncertainty sampling technique focuses its querying budget on refining the model’s classification boundary between the two initially labelled instances instead of exploring across its region of identically labelled areas diagonally across the plane. This can be overcome by adapting the query selection algorithm to balance the maximal informativeness coming from the informativeness function with another exploration utility measure. This interplay with informativeness measures, query selection, and their compositions — along with the considerations we have discussed above — give rise to the plethora of active learning strategies in literature and many yet unexplored avenues of research.
Table 5: IPAUC scores on balanced accuracy scores on a cold-start task configurations. Highest mean scores are bolded.

| Task Configuration          | Classification cold start IPAUC (balanced accuracy) |
|-----------------------------|----------------------------------------------------|
| UCI Parkinsons              | 0.7520±0.0752                                       |
| UCI Glass                   | 0.8275±0.0250                                       |
| UCI Seeds                   | 0.8885±0.0318                                       |
| Striatum Mini               | 0.9490±0.0000                                       |
| Gaussian Clouds             | 0.5087±0.0068                                       |
| Checkerboard 2x2            | 0.7253±0.0356                                       |
| Checkerboard 4x4            | 0.5110±0.0086                                       |
| Breast Cancer               | 0.8741±0.0145                                       |
| Synth Class 1               | 0.9799±0.0148                                       |
| Synth Class 2               | 0.9718±0.0093                                       |

Table 6: IPAUC scores on balanced accuracy scores on a warm-start task configurations. Highest mean scores are bolded.

| Task Configuration          | Classification warm start IPAUC (balanced accuracy) |
|-----------------------------|----------------------------------------------------|
| UCI Parkinsons              | 0.7645±0.0753                                       |
| UCI Glass                   | 0.9198±0.0347                                       |
| UCI Seeds                   | 0.8804±0.0524                                       |
| Striatum Mini               | 0.4980±0.0000                                       |
| Gaussian Clouds             | 0.6339±0.0067                                       |
| Checkerboard 2x2            | 0.7731±0.0228                                       |
| Checkerboard 4x4            | 0.5330±0.0153                                       |
| Breast Cancer               | 0.8942±0.0133                                       |
| Synth Class 1               | 0.9772±0.0058                                       |
| Synth Class 2               | 0.9959±0.0002                                       |

Table 7: IPAUC scores on mean square error on a cold-start task configurations. The lowest average mean square error is highlighted in bold.

| Task Configuration          | Regression cold start IPAUC (MSE)                  |
|-----------------------------|----------------------------------------------------|
| UCI Parkinsons              | 1.8077±0.0161                                       |
| UCI Glass                   | 13.3700±2.6240                                      |
| UCI Seeds                   | 1466.6133±71.6872                                   |
| UCI Energy                  | 533.9063±30.3188                                    |
| UCI Power                   | 194696.1155±59.6207                                 |
| Wine Quality                | 26.3305±0.9590                                      |
| UCI Tach                    | 191.1043±106.0610                                   |
| UCI Airfoil                 | 11391.2233±248.5694                                 |
| Diabetes                    | 574877.8421±28927.1300                              |

Table 8: IPAUC scores on mean square error on a warm-start task configurations. The lowest average mean square error is highlighted in bold.

| Task Configuration          | Regression warm start IPAUC (MSE)                  |
|-----------------------------|----------------------------------------------------|
| UCI Parkinsons              | 0.0922±0.1831                                       |
| UCI Glass                   | 15.1964±7.6292                                      |
| UCI Concrete                | 1418.5645±88.1003                                   |
| UCI Energy                  | 264.0951±21.3812                                    |
| UCI Power                   | 147479.2169±1249.972                                |
| Wine Quality                | 22.2955±0.6630                                      |
| UCI Tach                    | 84.8051±46.0703                                     |
| UCI Airfoil                 | 9407.7984±329.1265                                  |
| Diabetes                    | 78962.3416±1036.6245                                |
Figure 6: Plots of AL strategy performance on selected classification datasets,

Figure 7: Plots of AL strategy performance on selected regression datasets.