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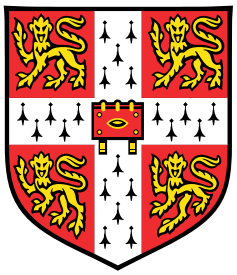

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This dissertation is submitted for the degree of
Master of Engineering

Robinson College May 2022

Declaration

I hereby declare that except where specific reference is made to the work of others, the contents of this dissertation are original and have not been submitted in whole or in part for consideration for any other degree or qualification in this, or any other university. This dissertation is my own work and contains nothing which is the outcome of work done in collaboration with others, except as specified in the text and Acknowledgements. This dissertation contains fewer than 10,000 words including appendices, bibliography, footnotes, tables and equations and has fewer than 40 pages.

Ross Brown
May 2022

Acknowledgements

And I would like to acknowledge ...

Abstract

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Nomenclature

Chapter 3

X_{test}	Datasets used to provide a score for the algorithms
X_{train}	Datasets used for training the algorithms
x_{known}	Data points where the true label is available to the algorithms used
x_{unknown}	Data points where the true label is not available to the algorithms used
y_{known}	True labels available to the algorithms used
y_{unknown}	True labels unavailable to the algorithms used

Chapter 1

Introduction

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Chapter 2

Previous Work

Scores displayed in examples have been based on the entire data set. Although this usually leads to data leakage within machine learning, this is not a concern here as the true comparison comes from testing *intelligent* vs *dumb* learning methods. In both of these cases, the model is kept identical, but the selection process in not. The baseline simply takes the first n entries from the data set, with the *intelligent* method described where required. Three data sets have been used to demonstrate on multiple data sets [][][].

2.1 Active Learning

There are several schools of thought regarding active learning. These can be separated into two distinct categories: current data and future predictions. The former of these is computationally cheaper, as will be apparent on description.

2.1.1 Current Data

Uncertainty Sampling

The simplest is applicable to cases in which a certainty is provided with each prediction. Settles [Set09] suggests selecting the data point with the largest uncertainty according to the current model. Using the dataset ”, this is demonstrated in Figure 2.1 with the algorithm for

deciding the next sample point given in Algorithm 1.

Algorithm 1: Uncertainty Sampling Selection

Data: X_{known}, Y_{known}, X_{unknown}
Result: Next X to label
model = BayesianRidge();
model.fit(X_{known}, Y_{known});
standard_deviation = model.standard_deviation(X_{unknown});
return *max(standard_deviation)*

As addressed by Settles [Set09], this can be extended to any probabilistic model.

$$x_{\text{next}} = \underset{X}{\operatorname{argmax}} \left[s_{g(X)} \right] \tag{2.1}$$

Settles [Set09] also notes the use of information theory for probabilistic models where y_i refers to all possible categorisations for x. This derives from the principle that the greatest entropy requires the most information to encode, and thus the least certain. However, Settles [Set09] fails to address non-probabilistic models in this instance, instead converting such models into probabilistic ones.

$$x_{\text{next}} = \underset{x}{\operatorname{argmax}} \left[-\sum_i P(y_i|x) \ln P(y_i|x) \right] \tag{2.2}$$

Broad Knowledge Base

A second form stems from information theory. Here, the aim is to produce an evenly dispersed x allowing a well-informed knowledge base. There are two paths to proceed: density and nearest neighbours.

The former of these requires a definition of density in a sparsely populated space. As an analogy, the density of a gas appears well-defined, it becomes non-smooth once the volume defined over is comparable to the distance between particles. Thus, a new definition is required.

Alternatively, nearest neighbour requires little explanation. x_{next} is the unlabelled data point furthest from any labelled data point.

$$x_{\text{next}} = \underset{x}{\operatorname{argmax}} \left(\sum \frac{1}{\operatorname{sim}(x, x_i)} \right) \tag{2.3}$$

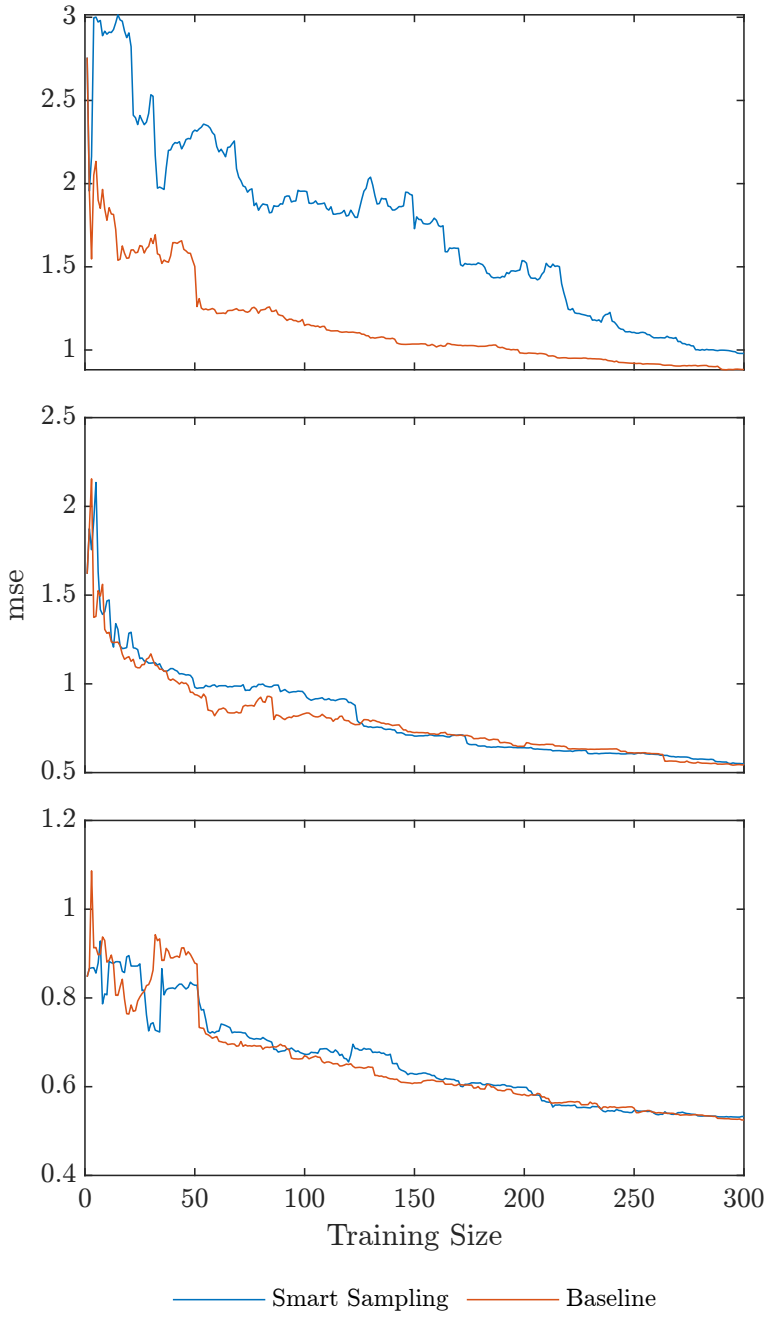
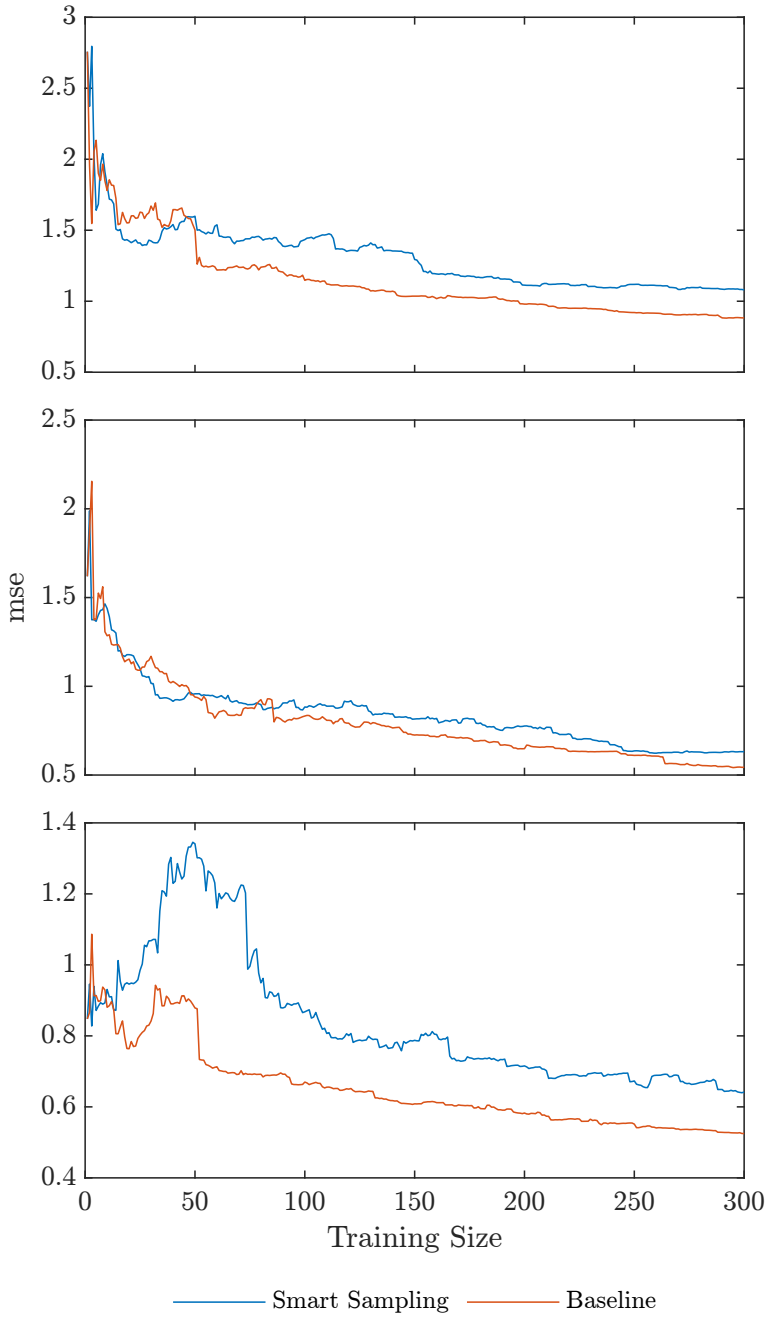


Fig. 2.1 boohoo



Density Hotspots

Conversely, a density weighted model has been suggested, as it escapes the introduction of error from outlier (i.e. data points far away from alternative data points). Settles and Craven [SC08] suggest (2.4) which can be broken down into two parts: a function for selection, ϕ_A, and a function for similarity, sim. The former arises from another method described in this section. The latter requires a function to describe the similarity between data points.

$$x_{\text{next}} = \underset{x}{\text{argmax}} \left[\phi_A(x) \times \left(\frac{1}{U} \sum \text{sim}\,(x, x_i) \right)^{\beta} \right] \tag{2.4}$$

Settles and Craven [SC08] admits that sim is open for interpretation. For simplicity, the average distance

Regions of Disagreement

As more complex methods are explored, we stumble across the method of competing hypothesis. This builds upon the [], and attempts to find []. The majority of work here relates to classification, although the same principles apply to regression. By minimising the region of disagreement between various models, a finer fit may be achieved.

One way of achieving this, especially in a regression model where boundaries are not quite so distinct, is to declare n models $M = \{m_1, \ldots, m_n\}$. Combining these allow for a model $\hat{m}$ to be defined with prediction $\hat{y}$, being the mean prediction of M, $\frac{1}{n}\sum y_i$ and a sample standard deviation $\hat{s}$ defined as the sample standard deviation of y_i. This standard deviation can be used as a measure of the disagreement between the models. Thus, using a method as in Section 2.1.1.

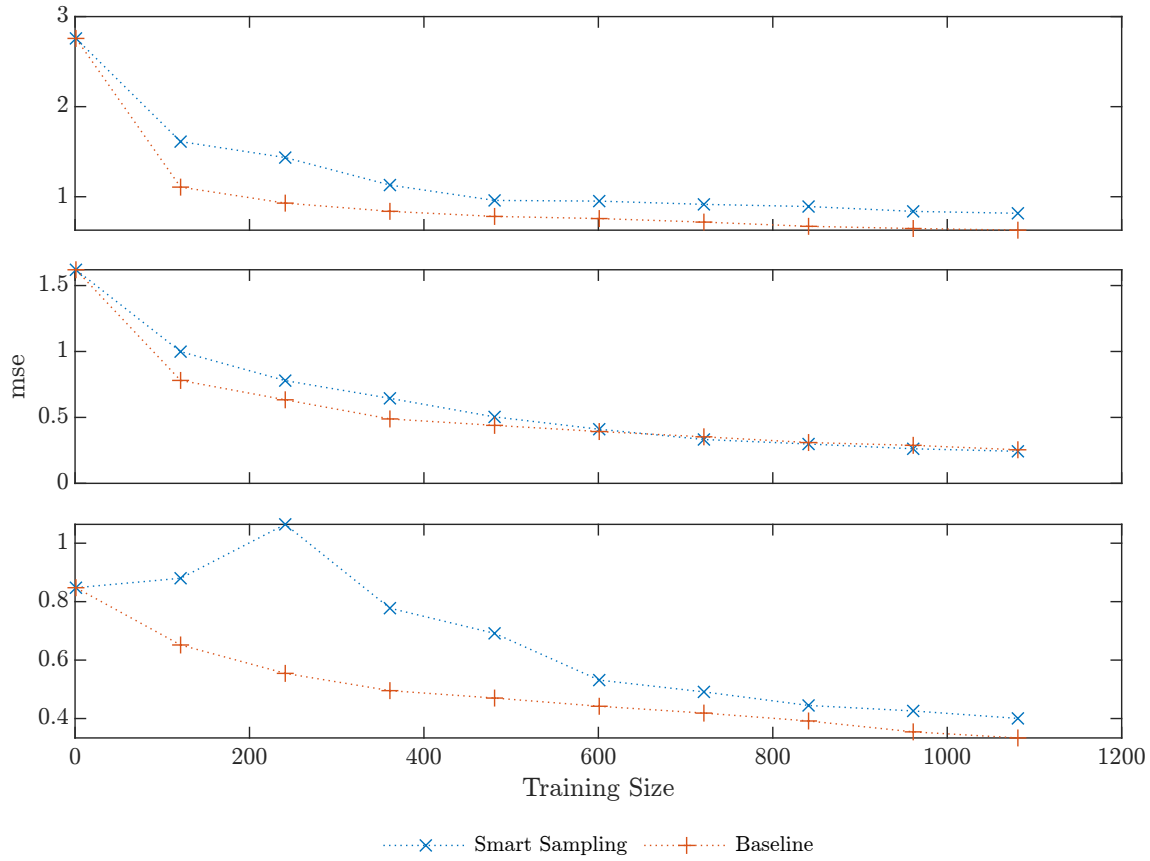
2.1.2 Estimated Future

These methods attempt to minimise a future attribute of the model. This works by predicting changes given with the inclusion of more data.

Expected Model Change

2.2 Batch Active Learning

Several naive methods are available here. Firstly, getting the top N data points from a model described in Section. However, this method does not take into account the equivalence of the data points. This is extremely clear using the highest uncertainty method. Each method in Section[] has been modified to demonstrate this weakness.


3
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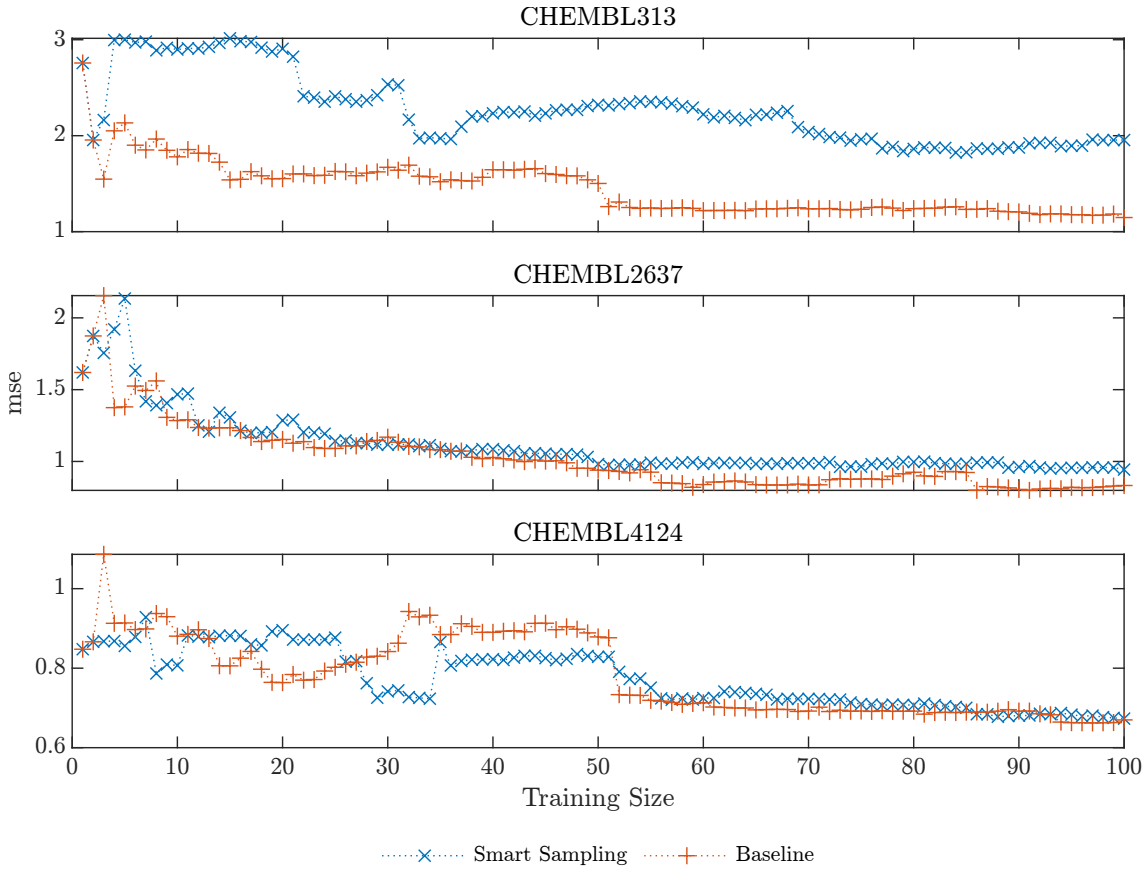
Training Size
Smart Sampling
Baseline



It stands to reason that the area which has the highest uncertainty will see this for the data points nearest neighbours. Thus, this singular data point suffers the potential of being surrounded by $N-1$ other data points. The benefit this provides in fitting the model is thus extremely limited, and only slightly greater than if one data point had been chosen. A simple fix would be to simulate the model after 1 iteration, and select the next point from here. By doing this $N-1$ times, a better solution may be found, although this may prove to be computationally very expensive.

2.3 Drug Data

There are numerous data categories that can be used to represent a chemical in a suitable form for machine learning. Each of these methods have various strengths and weaknesses. Some are directly based upon the chemical structure.

2.4 Physical Properties

A selection of physical properties from chemicals are known, from melting points to solubility. Many of these provide important aspects for consideration and allow human scientists to predict interactions, especially when determining new drugs. These data are often reported in tables within textbooks such as Perry's [] or provided through software [chembl ...]. Several of these data can be predicted through theoretical models, although the difficulty increases for larger molecules. For example, Lorem ipsum dolor sit amet, consectetuer adipiscing elit. Etiam lobortis facilisis sem. Nullam nec mi et neque pharetra sollicitudin. Praesent imperdiet mi nec ante. Donec ullamcorper, felis non sodales commodo, lectus velit ultrices augue, a dignissim nibh lectus placerat pede. Vivamus nunc nunc, molestie ut, ultricies vel, semper in, velit. Ut porttitor. Praesent in sapien. Lorem ipsum dolor sit amet, consectetuer adipiscing elit. Duis fringilla tristique neque. Sed interdum libero ut metus. Pellentesque placerat. Nam rutrum augue a leo. Morbi sed elit sit amet ante lobortis sollicitudin. Praesent blandit blandit mauris. Praesent lectus tellus, aliquet aliquam, luctus a, egestas a, turpis. Mauris lacinia lorem sit amet ipsum. Nunc quis urna dictum turpis accumsan semper.

2.5 Fingerprints

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2.6 Combining Drug Data with Active Learning

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Chapter 3

Methodology

3.1 Outline

The methodology presents a novel means of assessing different parametrised active learning methods on existing data sets, allowing for a robust answer into the use of active learning in drug rediscovery. Results can thus be given with a given belief. This approach has taken principles commonly used in machine learning and applied it to more traditional algorithmic methods.

Firstly, a collection of pre-existing data sets, X, are used. X is then split into two sub sets: X_{train} and X_{test}. Similarly to machine learning, the former of these subsets is used in fitting the parameters of the equation, and the latter is used to provide a result without the risk of data leakage into the training set. This is represented in []. Parallelisation is used to efficiently train the algorithms allowing the time for training to be $\sim \mathcal{O}(c)$.

Examining the smaller details, each algorithm is provided with the sets x_{known}, y_{known}, and x_{unknown}. Various algorithms are given these sets and allowed to generate a subset of x_{unknown} to be added into x_{known} alongside corresponding y_{known}. This can then repeat until a predefined stopping point is reached. Scores are reported using a weighted mean squared error [] based upon y_{predict} for all x. This is similar to a standard machine learning methodology with a couple of differences. Firstly, no distinction is made between the training and testing set within a dataset contrary to standard practice. This is due to two reasons. Firstly, the datasets are not large enough for an accurate representation of the data within the testing set, and secondly, the scoring to each dataset is not used within the machine learning algorithms to fit parameters as is usually the case. All algorithms used rely upon a simple custom composite model to allow for flexibility and consistency.

In Section [], it was discussed that there are various methodologies of representing chemicals and drugs. ... (if time)

3.2 Proof

In order to demonstrate the effectiveness, a few data sets are used instead, and the program is executed function by function. To start with, the underlying custom functions will be demonstrated, followed by the algorithms and then finally the training framework.

3.2.1 Custom Base Functions

Split

The split function allows for each dataset to be split into x_{known}, y_{known}, x_{unknown}, and y_{unknown}. This is required as a fundamental step for the algorithmic testing.

Repartition

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Model

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3.2.2 Active Learning Algorithms

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3.2.3 Training Framework

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Chapter 4

Results

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Chapter 5

Discussion

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Chapter 6

Conclusion

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