COAL: A Continuous Active Learning System

by

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Abstract

In this thesis, our objective is to enable businesses looking to enhance their product by varying its attributes, where effectiveness of the new product is assessed by humans. To achieve this, we mapped the tast to a machine learning problem. The solution is two fold: learn a non linear model that can map the attribute space to the human response, which can then be used to make predictions, and an active learning strategy that enables learning this model incrementally. We developed a system called Continuous active learning system (COAL).

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Chapter 1

Introduction

Businesses are constantly striving to improve old products or generate new ones. In many industries, performance measures for products are objective: the best graphics card runs the most computations per second, the best database provides the fastest queries, or the best television is the one with the highest definition. In this thesis, we focus on products for which performance is largely subjective: human assessment and preference is required in order to determine the superior product. These assessments can come in the form of a of rating (on a scale of 1 -5), a binary decision (like or dislike) and in some cases judgment as to whether or not a difference is noticeable[1]. This means that products require an evaluation that is far less mechanical, which makes the feedback and testing processes much more difficult.

The current method of generating new products: We are focused on problems where industry research departments tinker with multiple variables that make up the product in order to come up with a new one that, when assessed by humans, will surpass their current product in the metric of their choosing. This process relies primarily on the domain expert's knowledge of what may or may not work. The domain expert also has an understanding of the various constraints and underlying properties of the variables he or she has to work with, which could include:

- **How variables interact**: Some variables may interact with others and create

[1]This is the case with our sponsor, Coca Cola, where they are trying to find new coatings that do not change a product's flavor profile or taste experience

effects which might be detrimental to the intended goal.

- **Sensitivity**: Domain experts may have identified weak trends in the inputs and human responses. Experts may observe $x_1 \ldots x_k$ but notice that in particular, changes in x_1 and x_3 are easily noticed by humans.

- **Variable limits**: Domain experts also know the bounds within which each of the variable's values should fall. These bounds are often also dictated by external factors. For example, if it is a product that is consumed, there are certain limits on concentration for a given variable input.

While expert knowledge of variable interactions, sensitivities and constraints is extremely helpful, it still leaves a considerable amount of options for potential new combinations, and it is challenging to search through that space. Below, we describe a few of these challenges.

Challenges in searching through this space: While domain experts can create a defined feature space and use their prior knowledge to search for new combinations for products, there are limitations to what a business can do:

- **Cost**: The challenge of cost is broken into the *economic costs* and *time costs* that come with running experiments.

  Take economic costs: when running an experiment that requires human assessment, participants must be paid, and accommodations must be made in order to avoid confounding variables if any exist. Then, experts need to take their combination of inputs and synthesize many instances of the new product in order to get a large enough pool of responses to determine whether the new product is significantly better. All of this can incur a large cost, and must be done at each iteration of product testing.

  On top of that, for time costs, each step of the experimentation and human validation process may take a considerable amount of time. Time must be allocated towards generating new products. Additionally, it also takes time to gather a panel of humans to test the product. This results in human capital, which could otherwise provide benefits to a company in a different function, being locked up in the maintenance and continuation of a project.

- **Domain expert limitations**: Because industry scientists cannot try an endless number of combinations, they need to intelligently select the few that will give them an idea of what area in their feature space they should look in. However, domain experts are challenged as the dimensionality of the problem increases; that is, the challenge increases along with the number of variables they have to work with. While a domain expert may have intuitions regarding interactions among a few variables, and may be able to weakly postulate the human response, making accurate predictions becomes less feasible as the number of variables increases.

A potential solution using machine learning: In order to solve this problem using machine learning, one could fit a nonlinear model to determine the relationship between the available variables and the human responses – rating, like or dislike, judgment, or some other measure that establishes the product's success. Then, in a perfect setting where this relationship is accurately modeled, a user can search for the combination of variable values that results in the best product by predicting the human response using the model, instead of going to humans each time.

However, coming up with this accurate nonlinear model requires multiple steps and iterations.

1. Users must first start with a few data points, which can be sampled randomly or exist from prior experimentation.

2. Then, the existing few data points must be modeled to get a preliminary nonlinear model to work with.

3. From here, a user needs to identify valuable data points to improve the model *via* an approach called active learning or data points that will bring them closer to finding a better product, by optimizing the non linear model.

4. The user must then go out and synthesize a product from this combination of data points, and retrieve an aggregate response from a panel of testers.

5. The user then updates their model and repeats the process from step 3 to further improve their model and sample better products.

Ultimately, the result of this repeated process will create a model that allows a user to identify the best combination of inputs for his or her product without running countless human-in-the loop experiments.

1.1 Active Learning vs. our current scenario

Active learning is a field of study that looks to help researchers identify the data points that will best improve their models if provided labels. [6] In the past, active learning has worked well in areas such as image classification on image data and sentiment classification on text data. [5] [20] There are numerous image datasets with labels with which to conduct preliminary training of a classifier. Even without a substantial amount of initial data, users can hire mechanical turks and acquire a sizable base to train on for a relatively low cost due to the nature of tagging image data.

From here, users have enough data to begin making predictions on unlabeled data in order to identify the most valuable data for their models using active learning methods. [21] The same is true for sentiment analysis of text data. While there are not as many text datasets with labels, and sentiment analysis does take more time, data labeling can be done remotely in relatively little time. Then, users can repeat the same process of building models and beginning to identify informative unlabeled data for labeling.

In this thesis, we consider a slightly different problem where human assessments cannot be collected *remotely* or *digitally.*

Our use case is that of sensory evaluation. In sensory evaluation, humans either taste, smell or touch new products in order to assess them. These new products could involve flavors or fragrances. These experiments require the physical presence of the human assessor and cannot be done digitally. Additionally, they require much more control than other types of evaluation to avoid erroneous results. In the instance of image classification, external factors such as health, mood, or other sources that can influence a person's subjectivity will not impact a person's ability to recognize objects like a dog in a picture. However, that is not the case in sensory evaluation. The evaluation is often done in a controlled setting to account for environmental factors.

A perfect example is the unique problem provided to us by Coca Cola. Coca Cola is interested in changing the coatings on the insides of their cans, but they do not want the customer to taste a difference. In similar scenarios where companies are looking to change a consumed product, firms take multiple steps to carefully ensure that there are no confounding variables or measurement errors. Panelists of consumers are brought on-site to avoid confounding variables and are given food to cleanse their pallets after trying each sample, and results are meticulously kept. As one can see, each iteration requires a substantial amount of time for generating new samples and testing, and even with these precautions, a company can only run so many tests before the panelists' sensitivities to taste are potentially dulled. Therefore, our problem is slightly more nuanced than most, and requires further thought before using an active learning solution.

1.2 What are the constraints?

Let us consider, then, the unique hurdles that sensory evaluation presents for the development of an active learning solution.

- **We do not have many points to start with.** To begin with, we do not have many data points to develop, test and validate a machine learning model. Without this we cannot start with a non-linear model.

- **We cannot ask for more data points.** Given the lack of data points, we explored if we could gather more. In the time frame we set for this project, however, it is unlikely that we could do so; experiments take time.

Yet our goal is to develop and deliver a machine learning system that is capable of performing the 5 steps mentioned above in the first section under "*A potential solution using machine learning*". Hence, we examined: if we were given enough data, what questions could we ask in order to deliver a good system? There are three questions we would have sought to consider:

1. **Which machine learning model best fits the data?** There are many different modeling techniques with different ways of modeling non-linearities. We would have asked which non-linear model best fits this type of data.

2. **Which active learning method is best?** As with the above, and with a lot of labeled data, we would have asked which one of numerous techniques would work best for this problem.

3. **Does active learning help?**: We would have asked whether an active learning loop would help in this context.

1.3 A continuous active learning system

We thus developed a continuous active learning system (COAL) as an answer to industry's need to navigate unlabeled data efficiently and cost-effectively. We take in all of the considerations and predispositions mentioned above in order to create a system that allows a user to leverage machine learning to model the data that he or she does have and to search this space.

In order to address a lack of data to begin with, we attempt to ensure the robustness of machine learning models and active learning methods chosen to embed in COAL. We run thousands of simulated active learning experiments that test a variety of nonlinear models for a variety of different human assessment functions that we create through "ground truth" models.

Then, we evaluate active learning methods in a similarly simulated process to determine whether or not active learning will actually help given our problem and, if it does, which methods are the best for this type of learning scenario.

Ultimately, the user is provided the most robust modeling technique as well as an active learning strategy, as assessed from these experiments, that is integrated into a series of modules. These modules allow the user to model their data, predict the response from a combination of inputs, and intelligently propose new queries for labels. This way, after enough initial experimentation and human testing, a user would be able to accurately model the function that drives human assessment and infinitely test new products without the costs that are typically associated with that process.

1.4 Thesis Roadmap

The remainder of the thesis is organized as follows:

Chapter 2 introduces how machine learning is used, one of the major challenges that modelers face, the models we test, and successful use cases.

Chapter 3 talks about how active learning is used, some of the strategies, and past successes.

Chapter 4 discusses the COAL system and its primary components at length, and introduces an end-to-end explanation of its use. Chapter 5 runs through the process of how we go about simulating active learning experiments and the results of these simulations. Finally, Chapter 6 reviews key findings, identifies the core contributions of this work, and provides insight into what future work will look like.

As a whole, this thesis introduces a system for running active learning in non-traditional active learning settings.

Chapter 2

Non-Linear Modeling

One of the core components of the solution is the non-linear model, which is the user's attempt at recreating the actual underlying function that determines a human's response. The non-linear model does what a domain expert cannot by capturing higher-dimensional relationships, and providing a more analytically sound method of making forecasts on the outcomes of testing given a combination of variables. As a result, many companies are currently taking advantage of machine learning in tasks that can be systematically broken down, and where basic human discretion can be substituted with statistical forecasts.

Overview of using machine learning: Many resources have been created that allow users to easily train and utilize machine learning models in a variety of languages. The following provides a basic understanding of how machine learning models are built, and how they function:

1. **Prior to training**: Prior to training, machine learning models comprise a series of assumptions about the data, adjustable weights or kernels, and an algorithmic framework through which the function inputs pass through.

2. **Training the models**: Training machine learning models focuses on finding a set of parameter weights that, when combined with the model assumptions and the algorithmic framework of the model, provide an output close to the actual observed process. This process may be thought of as a user going back

and forth between inputs and outputs by tweaking the weights of the model so that, if the same inputs were ever provided in the future, they would provide the same corresponding outputs.

3. **Using the model after training**: The primary function of using a machine learning model after training is to forecast the output of a new set of inputs.

The model selection problem: One of the main problems in machine learning is determining the model that best captures the relationship between the input variables $x_1 \dots x_k$ and the response variable y. These models, to list just a few, include random forests, support vector machines, Gaussian processes, and neural networks, all of which make different assumptions about the data and model the data in substantially different ways. In most modeling scenarios, the user has a sizable pool of data to model from. The benefit of having this pool is that a user can fit a wide variety of models to the data to determine which achieves the best accuracy or is the most robust. A large pool of data allows the user to run various forms of cross-validation, and modelers can use multiple different model selection methods to determine which model is right for the task. Sadly, we do not have a large enough initial pool of data; hence, there is no way for us to explore various models, simply because there will not be enough instances to draw any conclusions with conviction. Therefore, we are required to make different considerations in our model selection process, and run tests as specified in Section 5 in order to choose the most robust model for all cases as opposed to a model that would be a best fit for a given application.

2.1 Machine Learning Models

In this thesis, we focus primarily on two classification methods with the capacity to capture highly non-linear relationships between data points and a response variable. The two models that we focus on are Gaussian process classifiers and neural networks.

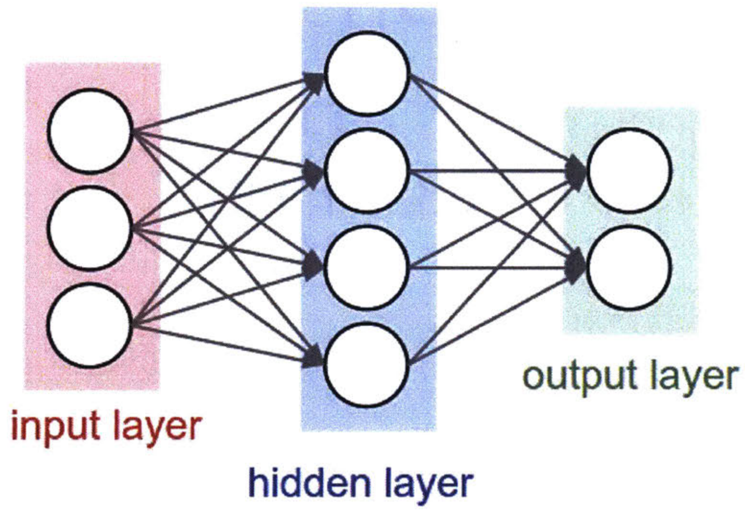


Figure 2-1: This graphic depicts a basic neural network which takes 3 inputs through the input layer, propagates these inputs through the hidden layer, and outputs probabilities of each pre-specified class in the output layer.

2.1.1 Neural Networks

Neural networks are a very powerful type of nonlinear classifier that have grown in popularity due to recent strides in areas such as computer vision and natural language processing (we have even found instances in which researchers used neural networks in conjunction with sensory analytics [23]). A neural network is generally characterized by an input layer, a hidden layer which is its defining feature, and an output layer where label probabilities are outputted. Another way to think of neural networks is as a series of layered logistic regression functions. At each node of the neural network, multiple inputs are provided and go through a sigmoid function, just as they would in a logistic regression. The difference is that neural networks take the outputs of the initial nodes or sigmoids and use those as inputs to additional logistic regression functions. This ultimately results in a highly nonlinear classifier that is able to capture a variety of different functions.

2.1.2 Gaussian Process Classifiers

The second nonlinear classification model that we consider is the Gaussian process classifier. This model is also able to robustly capture nonlinear relationships. The

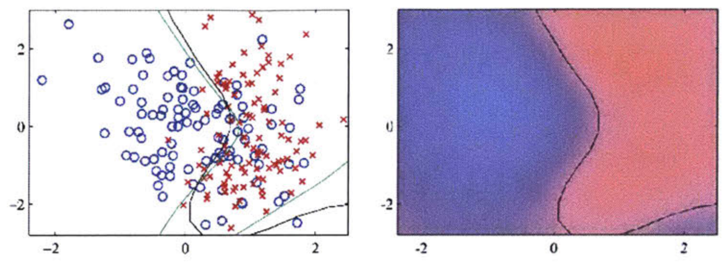


Figure 2-2: This graphic depicts an instance of the type of boundary that Gaussian Process Classifiers create when fitting data. [1]

Gaussian Process Classifier is non-parametric and specified by its mean function and covariance function. Perhaps one of the easier-to-understand explanations of Gaussian Processes can be found in Murphy's *Machine Learning: A Probabilistic Perspective*:

> A GP defines a prior over functions, which can be converted into a posterior over functions once we have seen some data. Although it might seem difficult to represent a distribution over a function, it turns out that we only need to be able to define a distribution over the function's values at a finite, but arbitrary, set of points, say $x_1 \dots x_N$. A GP assumes that $p(f(x_1), \dots, f(x_N))$ is jointly Gaussian, with some mean $\mu(x)$ and covariance $\sum(x)$ given by $\sum_{ij} = k(x_i, x_j)$, where k is a positive definite kernel function. The key idea is that if x_i and x_j are deemed by the kernel to be similar, then we expect the output of the function at those points to be similar, too. [11]

The Gaussian Process is then funneled through a sigmoid function which, just as it does in logistic regression, turns the problem from a regression problem into a classification problem.

2.1.3 Modeling with a Human Component

While it may seem overly complicated to model the behavior or abilities of people given that each person is unique, at an aggregate level, scientists have found that there are patterns that persist. Companies such as Netflix are able to create recommender systems that identify human preferences and provide suggestions on what the person may want to watch next. [22] Researchers are also capable of identifying the content of images with a high degree of accuracy. [10] What these successes in machine learning mean is that any process can be modeled and to a high degree of accuracy even when something as fickle as a human is involved. However, at the end of the day, these models are only frameworks and are as good as the data they are trained on which brings us to Section 3.

Chapter 3

Active Learning

The active learning problem is best known as a situation where a modeler wishes to identify a relationship between a set of input variables $x_1 \ldots x_k$ and a response variable y but has largely unlabeled data. The alternative scenario is a branch of machine learning called supervised learning where the user receives input values for each variable $x_1 \ldots x_k$ and also receives the actual outputs y for those values. This scenario is far more common because it does not require much discretion in the gathering of data points. However, in active learning, usually due to some cost of labeling or gathering each response value y, researchers attempt to formally capture the relationship with the fewest labels y.

The active learning process: In active learning, the process is composed of two main constituents: the oracle and the modeler. The oracle is an omniscient labeler who is capable of providing a label for any combination of inputs asked for by the modeler. However, each request for a label comes at some cost. In order to minimize the cost, the modeler uses his or her model that has been trained on the data he or she does have labels for, the unlabeled data, and active learning methods to identify valuable or informative data points. After each query is made to the oracle, the modeler updates the trained model which brings it closer to the true relationship between the input variables and the response variable. From here, the modeler repeats this process to continually improve the accuracy of the trained model.

3.1 Active Learning Methods

There are a wide variety of ways to determine whether a given unlabeled data point is informative. Information can come from the nature of the data itself if there are clusters or certain structures such as multiple levels of clustering. A modeler can also look at the model he or she is using as well to determine what could potentially be helpful for capturing the relationship in the data. He or she could see if the model believes that two classes are equally probable or whether or not updating the model with a given data point and label would reduce the overall prediction error.

The methods that we explore for the COAL system at this current time are primarily the single-query methods that are well established throughout active learning literature. They are *smallest margin* and *entropy*. These methods are generally well understood and fairly easy to interpret given their simplistic nature. The process to use these methods is as follows:

1. As a modeler, you begin with your labeled data X and labels Y.

$$X_{labeled} = \begin{bmatrix} x_{11} & \dots & x_{1N} \\ \vdots & \ddots & \vdots \\ x_{M1} & \dots & x_{MN} \end{bmatrix} \quad \text{and} \quad Y_{labeled} = \begin{bmatrix} y_1 \\ \vdots \\ y_M \end{bmatrix}$$

2. You then train your classification model $f(x) = y$.

3. From here, you predict the probabilities of each class C for all 1 to K classes on all unlabeled data points.

$$X_{unlabeled} = \begin{bmatrix} x_{11} & \dots & x_{1N} \\ \vdots & \ddots & \vdots \\ x_{M1} & \dots & x_{MN} \end{bmatrix} \Rightarrow f(X_{unlabeled}) = \begin{bmatrix} p_1(C_1) & \dots & p_1(C_K) \\ \vdots & \ddots & \vdots \\ p_M(C_1) & \dots & p_M(C_K) \end{bmatrix}$$

4. Next, the user can choose to use *smallest margin* or *entropy* to determine the next query.

For smallest margin [14]:

(a) For each row, find the two highest probability values and calculate the difference Δ between the two values.

(b) Append each delta to a list called Margin.

$$Margin = \left[\Delta_1 \ldots \Delta_M\right]$$

(c) Now, sort the list from lowest to highest in descending order and select the top query to propose by finding the index corresponding to the actual combination of inputs x found in $X_{unlabeled}$.

For entropy [19]:

(a) For each row, calculate the entropy of $f(X_{unlabeled})$ as $en_m = \sum_{n=1}^{K} p_{mn} log_2(p_{mn})$.

(b) Append each entropy value to a list called Entropy.

$$Entropy = \left[en_1 \ldots en_M\right]$$

(c) Now, sort the list from highest to lowest in descending order and select the top query to propose by finding the index corresponding to the actual combination of inputs x found in $X_{unlabeled}$.

On a last note, another strategy that we will refer to is the "Random" uncertainty sampling strategy. Random is essentially how supervised learners will sample data or those that use little to no discretion in determining what data is more informative. To use this method, one just randomly selects a data point from the existing data pool. This is what we consider as the benchmark for the efficacy of the active learning strategies.

3.2 Active Learning Successes

In recent years, active learning has grown in popularity due to a widespread interest in determining whether or not machine learning can solve a variety of problems in industry. Some of the potential benefits that users of active learning are looking for are:

- **Reduction of Costs**: This factor is key, because companies are limited in the amount of time and money they have to create a new product. Also, there is a competitive edge for those who are able to generate a product faster.

- **Training Time Reduction**: Although GPU computation has improved substantially in the last decade, modelers are still looking for means to cut down on the amount of time it takes to train a model. In [21], training a deep neural net for image classification took 17 hours with a Titan X GPU for 44,708 images which was one of the fastest commercial graphics cards available at that time. Even with the computational improvements since then and the ability to run calculations in parallel, researchers are limited in the complexity of the model that they can train. Therefore, modelers are hoping to reduce the training data sets to at least gain some reduction in the amount of computation required in order to achieve the same accuracy results as one would get if training on all of the data available.

- **Improving Existing Classifier Accuracy**: Finally, a third application for active learning is also for the sake of further improving models. While many modelers are able to capture the more robust features of the classes that they are trying to identify in image data and so on, their models still tend to suffer in edge cases. This is another area where, even after one has fully trained a model, active learning can still provide a level of benefit by capturing rare or unusual cases to learn a model from.

Proof of Active Learning Success: At this point, active learning has definitively proven its value across multiple applications in literature. Drawing once again from

[21], researchers were able to train a deep learning model with slightly above 60% of the the CACD dataset [4] that was carefully chosen using active learning and achieved a similar accuracy rate to a supervised learner who used the entire dataset to train the same model. Then, in [3], researchers used Gaussian mixture models with active learning on the VidTIMIT [7], a video and audio dataset, and MOBIO [13], a biometric dataset. In both cases, active learning methods performed much better than the supervised learning benchmark of randomly selecting data points to label. In some cases, the active learning methods allowed the modeler to achieve the same accuracy as the supervised learner but having trained on half the number of data points. There is a great deal of interest in how the data collection process can help researchers create better models with fewer labeled data points.

Chapter 4

COAL: A continuous active learning system

To reiterate, the problem that COAL aims to tackle is the scenario where a modeler is trying to determine the most informative data points in order to build a model that is representative of the underlying data generating process. This process is generally unknown to the domain expert or user and, at most, users generally have an idea of constraints only but not much more. COAL's objective is to take this problem and map it to a learning problem through the use of active learning strategies and machine learning models. COAL's framework allows users to continually query for data points in order to find informative data points and continuously improve the accuracy and conviction of their models.

4.1 Modeler, Predictor, Proposer Framework

The COAL system has three components.

1. **Modeler**: The *modeler* models the latest available data samples. In our case, these data samples are the input variables $x_1 \ldots x_k$ and the aggregated response from the human panel. To model this data, we chose two different types of modeling techniques: neural networks and Gaussian process modeling.

2. **Predictor**: The *predictor* module allows the user to propose a new combination of variables and receive two prediction outputs. The first prediction will be the label that the model believes that the data point has and the second value will be the probability that the model assigns to the likelihood of it being the "detected" label.

3. **Proposer**: Using the active learning methods we developed, the *proposer* suggests the next combination of input variables to try by proposing attributes, which the user can then experiment with. The proposer uses the latest model and the data from the past experiments to come up with new data to query. The *proposer* then creates a number of data points by generating values for attributes $x_1 \dots x_k$ and by stepping through the multidimensional space with a step size s. This will create $\Pi_{i=1}^{k}|\frac{max(x_i)-min(x_i)}{s}|$ possible input combinations. Next, we pass all these candidates through the up-to-date model. The model, in turn, provides the likelihood probability for each of the input combinations to succeed in human panel testing. Our goal is to pick a candidate from these. In order to maximize exploration of the space, we use two methods such as *smallest margin* and *entropy* to pick a candidate[6]. As a result of querying informative samples, we have a higher potential for more consistency and improvement in accuracy of our model as new samples are labeled and added to the model.

4.2 Running Active Learning Iterations

Now that we have outlined the core components of the COAL system, we go into detail on how one would run active learning iterations. The COAL system is to be used in the following manner:

1. The user provides preliminary data with labels, model type, and model hyperparameters to the Modeler function.

2. The Modeler function trains the selected model on the provided data.

3. The Modeler function creates a "Trained_Model.pkl" file which is saved to the current working directory.

4. The Modeler function outputs the current model to be used in further components of the COAL system.

5. From here, users are able to leverage the model to gain access to the predictor and proposer functionalities and would start with the Predictor function.

6. To use the predictor, the user provides inputs for each variable and then clicks predict. This allows a user to formulate potential queries and compare with the current model to see if the model agrees with his or her intuition. In many cases, these potential query designs can come from different analytical methods.

7. Now, the user moves on to the Proposer function and provides the trained model which was created using Modeler, the number of variables, the minimum ranges for each variable, the maximum range values for each variable, the step sizes to be observed between each minimum and maximum value, the active learning method, and the number of queries.

8. The proposer then consists of three sequences that occur in the following order:

   (a) The proposer makes a call to an internal function called "Data Generator". The Data Generator function takes the trained model, number of variables, minimum range values, maximum range values, and step sizes in order to generate a range of data point combination defined by the inputted values. For example, if I have 1 variable, a minimum range value of 0, a maximum range value of 10, and a step size of 2, the outputted data will be [0,2,4,6,8,10].

   (b) The proposer then has the trained model predict on the entire array of input values that were created by the Data Generator function. The result of these predictions are a series of probabilities for each provided label class.

(c) Finally, the proposer makes a call to one of the active learning strategy functions depending on the active learning method parameter provided to the proposer function. The active learning function will return informative queries based on the probabilities provided and the number of queries requested.

9. The proposer then outputs the informative samples for the user to take to an external oracle for the labels to be queried.

10. Once the labels have been identified for the informative samples, the user is to add these data points along with their labels to the respective input X and label Y arrays.

11. Now, since the data has been updated and there is new data to train on, the user will once again call Modeler to update the model based on the new information provided.

12. The user repeats steps 6 - 10 continuously in order to further explore the feature space until generally an external constraint such as an economic stopping criteria is applied.

4.3 COAL User Interface

Additionally, we developed a front end application for users without programming experience to gain access to COAL. The following steps provided will guide a user through the active learning process via this interface. Much of this process is similar to Section 4.2 but with a few nuances that are specific to the user interface. The steps are as follows:

1. The user is prompted for the number of variables which is saved in the back end.

2. The user is prompted for the variable names to carefully track what values correspond to what ingredients or actual variables in the experiment.

3. The user then goes to the Modeler page which has four different windows. One for Panelist responses, one for ingredients, one to model the data, and one to download the training data so far.

4. The user clicks on the upload button under ingredients in order to upload an "Ingredients.csv" file.

5. The user clicks on the upload button under the panelist responses in order to upload a "Panelist_Responses.csv" file.

6. Then, the user clicks the "Model" button under the Modeling section. Behind the scenes, the chi-square test is calculated for the panelist responses to determine the aggregate response of the panelists. Then, the ingredients and aggregate responses are joined and appended to the "Training_Data_So_Far.csv". Finally, a model is trained based on the ingredients or variables and the responses in the "Training_Data_So_Far.csv" file.

7. From here, the user can move on to other modules. Next, a user may proceed to the Predictor module.

8. The user provides inputs for each variable and then clicks predict. This allows a user to check to see what the model thinks about various combinations of potential inputs. This stage is where the user can evaluate certain priors based on application based knowledge and further validate or question his or her hypothesis of viable data points to label.

9. Next, the user can go to the Proposer module which will allow him or her to take advantage of active learning strategies. The user supplies the maximum value constraints, the minimum value constraints, the step size, and active learning method in order to get a proposed combination of variables.

10. The user would then synthesize a product from these combinations of variables and test them in order to generate more responses for a "Panelist_Responses.csv"

file. Furthermore, the researcher would input the combination of variables into another "Ingredients.csv" file.

11. Finally, the user would go back to the Modeler page and repeat the process from Step 3 with the new "Ingredients.csv" and "Panelist_Responses.csv" files.

Chapter 5

Robustness Experiments

In traditional machine learning, data collection is often trivial, and data scientists are able to hire mechanical turks [8] to collect thousands of data points to build initial models. This allows them to try a wide variety of models such as neural networks, random forests, support vector machines, and many more to determine which model is the best for the task at hand. Since we want to address situations with no or minimal data in this thesis, we need to devise a means of testing viable models for robustness so that, when the data is introduced, the model is able to capture all of the underlying nuances and variations.

Second, this relatively substantial pool of initial data also allows the best model to begin to robustly capture some of the underlying relationships in the data. Researchers have found that active learning, which tends to focus on unclear or "hard to identify" examples without a base of "easy to identify" data points, can confuse a model into failing to create robust decision boundaries [2]. Therefore, in this section, we also seek to answer whether or not active learning helps in our scenario and, if multiple models are helpful, which one is the most robust.

To answer these questions, we begin by coming up with different variations of nonlinear ground truth models to replicate what the data might look like. In Section 5.1, we describe the steps necessary to create each ground truth model, and go through what can be varied in the process. Then, in Section 5.3, we address the machine learning model selection process. In this section, we select a model, run many simulated active learning experiments with various ground truth models, and collect the aggregate statistics of our evaluation metric which is introduced in Section 5.2. This provides us with an expectation of how a model should perform when used in a real experiment. Next, in Section 5.4, we simulate many active learning experiments again, but vary the active learning methods. This generates insight into what active learning methods perform the best overall, and into which models a particular method performs the best with. Finally, we evaluate the variance of our evaluation metric in order to determine the most robust models and methods. We look for the lowest variance in performance across many iterations in order to find the most robust model and active learning method.

5.1 Generating Ground Truth Models

The ground truth model is an essential component to replicating the active learning process because it acts as the data labeler or "oracle" as mentioned in Chapter 3. Throughout our testing of the active learning process, when an active learning strategy has identified an informative data point, the modeler queries the oracle for a label for that data point. Furthermore, in literature [9] [15] [17], researchers have found that different strategies perform better for different applications. Therefore, it is imperative that we systematically define the ground truth model generating process in order to generate insights on how training models and active learning strategies interact when the underlying process is driven by one type of oracle model or another.

The ground truth model generating process is broken down into the four steps, as described below:

1. **Generating Ground Truth Data**: To generate the ground truth model, we start by using scikit-learn's make_classification function, which creates clusters of data points with labels based on a series of inputs listed below.

    - **n_samples**: This determines the number of samples that the function will generate.

- **n_features**: This parameter determines the number of features that will be created in the resulting input variable matrix X.
- **n_informative**: This parameter will determine the number of variables that are actually informative relative to the response variable.
- **n_redundant**: This parameter will create redundant variables that are meant to create collinearity.
- **n_clusters_per_class**: This parameter determines the number of clusters that are generated per class.
- **n_classes**: This parameter determines the number of classes that will be created in the response vector y.
- **class_sep**: This parameter determines the distance of one cluster from another. The larger the class_sep value, the more distant the clusters are from each other, and the easier the classfication problem becomes.

Ultimately, the output of this function is an input X matrix with N variables and M data points and a response vector Y with M data labels which abides by the parameters provided.

$$X = \begin{bmatrix} x_{11} & \dots & x_{1N} \\ \vdots & \ddots & \vdots \\ x_{M1} & \dots & x_{MN} \end{bmatrix} \qquad Y = \begin{bmatrix} y_1 \\ \vdots \\ y_M \end{bmatrix}$$

2. **Pick Model Type**: The next step is to choose the model that determines the relationship between the X input values and the Y response variable. There is an extensive list of different machine learning models that make different assumptions, have their own limitations, and capture nonlinearities in their own specific way. A few examples include:

   - **Decision Trees** which map predictors to the predicted variable by splitting the feature space repeatedly until the majority of data points after several splits belongs to just one class.

Ground Truth Model	Hyperparameter	Explanation
Neural Network 1	hidden layer size = (100,)	One layer, 100 nodes
Neural Network 2	hidden layer size = (30,30)	2 layers, 30 nodes each
Neural Network 3	hidden layer size = (20,20,20)	3 layers, 20 nodes each
GP Classifier 1	kernel = 1.0*RBF(1.0)	radial basis function, length_scale 1.0
GP Classifier 2	kernel = 2.0*RBF(1.0)	2*radial basis function, length_scale 1.0
GP Classifier 3	kernel = 5.0*RBF(2.0)	5*radial basis function, length_scale 2.0

Table 5.1: Ground Truth Model Hyperparameter Arguments

- **Neural Networks** which consists of a series of layered logistic regression functions. In image data, neural networks can capture the edges in images and use additional functions such as "convolution" to combine edges into outlines of the faces of dogs, cats, and people.
- **Support Vector Machines** which look for the separating hyperplane that maximizes the distance between two classes.
- **Gaussian Process Classifier** which uses approximations to determine the most likely Gaussian function based on the observed data points, and then passes those values through a sigmoid function to make classification predictions.

3. **Pick Hyperparameters**: After the model is chosen, there are multiple hyperparameters in each model that can be tinkered with. In the ground truth models that we pick, the hyperparameter selection are shown in Table 5.1.

4. **Train Model**: At this point, a user is ready to create a ground truth model. He or she will:

   (a) Take the data created from scikit-learn's make_classification.

   (b) Retrieve the model and the model hyperparameters.

   (c) Train or fit the model in order to create the ground truth model.

5. **Collect and Save Model**: Finally, the user should collect and save the model. In Python and scikit-learn, models are saved through a Pickle file in sklearn's "externals" subpackage.

n_samples	1000
n_features	2
n_informative	2
n_redundant	0
n_clusters_per_class	1
n_classes	2
class_sep	3.0

Table 5.2: Scikit-learn Make_Classification Arguments

For the experiments that we run, we create ground truth models with the following parameters.

1. We selected the parameters for the scikit-learn make_classification function from Table 5.2.

2. Then, we picked the Gaussian Process Classifier and Neural Networks as our desired ground truth models.

3. Finally, we chose the hyperparameters as listed in Table 5.1.

As a result, we developed 6 highly nonlinear models to act as the ground truth for the experimental results in Section 5.3.

5.2 Simulating Active Learning with an Oracle

Next, since we create various ground truths through training nonlinear models, we are able to simulate active learning without real data. These active learning iterations are depicted in Algorithm 1 from lines 6 to 11. The oracle provides the labels in response to a query, the queried data is appended to the model training set, the model is trained, and finally a new query is generated through active learning.

```
Algorithm 1: Active Learning with an Oracle
Input  : Active Learning Iterations $I$, Maximum Range values $Max_v$,
         Minimum Range values $Min_v$, Stepsize values $S_v$, Number of
         Variables $v$, Initial Number of Data Points $I_0$, Number of Queries $N_Q$
Output: mean and standard deviation of $C^E$
1  Pick an untrained model $f_R$ for robustness testing.
2  Pick an active learning method $AL$.
3  $X_{all} \leftarrow$ Data_Generator($v$, $Max_v$, $Min_v$, $S_v$).
4  $X_{Query} \leftarrow$ randomly sample $I_0$ data points from $X_{all}$.
5  Initialize $X_{TRAIN}$, $Y_{TRAIN}$, $Accuracy_i$ as empty matrices.
6  for $j = 0$ to $I$ do
7      $Y_{Query} \leftarrow f_{GT}(X_{Query})$.
8      Append $X_{Query}$ to $X_{TRAIN}$ and $Y_{Query}$ to $Y_{TRAIN}$.
9      Train $f_R$ on $X_{TRAIN}$.
10     $X_{Query} \leftarrow$ Proposer( $f_R$, $X_{ALL}$, $AL$, $N_Q$).
11 end
```

Now that we have the ground truth model to query labels from, the remaining component is the Proposer which comes up with the actual queries. The Proposer's functionality is explained in Algorithm 2 and utilizes the active learning methods that were discussed in Chapter 3.

Algorithm 2: Proposer Function

```
Function Proposer($f_R$, $X_{ALL}$, $AL$, $N_Q$):
    $Class\_Probabilities \leftarrow f_R(X_{ALL})$
    $Indices \leftarrow AL(Class\_Probabilities, N_Q)$
    $X_{Query} \leftarrow X_{ALL}[Indices]$
    return $X_{Query}$
Function Smallest_Margin($Class\_Probabilities$, $N_Q$):
    Initialize Margin as an empty list.
    for $i = 0$ to $length(Class\_Probabilities)$ do
        $max_1 \leftarrow$ is the 1st largest class probability
        $max_2 \leftarrow$ is the 2nd largest class probability
        $\Delta_i \leftarrow max_1 - max_2$.
        Append [ $\Delta_i$, $i$ ] to Margin.
    end
    $Margin \leftarrow$ Sort($Margin$) by $\Delta$ in ascending order.
    return first $N_Q$ values in the $i$ column from Margin
Function Entropy($Class\_Probabilities$, $N_Q$):
    Initialize Entropy as an empty list.
    $K \leftarrow Number\ Columns\ in\ Class\_Probabilities$
    for $i = 0$ to $length(Class\_Probabilities)$ do
        $en_i = \sum_{n=1}^{K} p_{i,n} log_2(p_{i,n})$.
        Append [ $en_i$, $i$ ] to Entropy.
    end
    $Entropy \leftarrow$ Sort($Entropy$) by the $en$ column in descending order.
    return first $N_Q$ values in the $i$ column from Entropy
Function Random($Class\_Probabilities$, $N_Q$):
    Initialize Random as an empty list.
    Append $N_Q$ randomly sampled values from
      1 to $length(Class\_Probabilities)$ without replacement to Random.
    return Random
```

5.2.1 Evaluation Metric: Area under the Accuracy Curve

One of the unique benefits that we get with the ability to assume a ground truth model is that we can infinitely query our own oracle. This luxury is not available in the real world and is generally not considered. The are two main benefits to this:

1. For any ground truth model we generate, we can exactly determine our training model's accuracy relative to the ground truth. Whether we decide to expand the constraints or severely reduce the stepsize values, additional data collection outside of the original dataset comes at no extra cost.

2. Also, since we create the ground truth model, we know that a robust enough model should be able to converge perfectly to the ground truth model if given enough data.

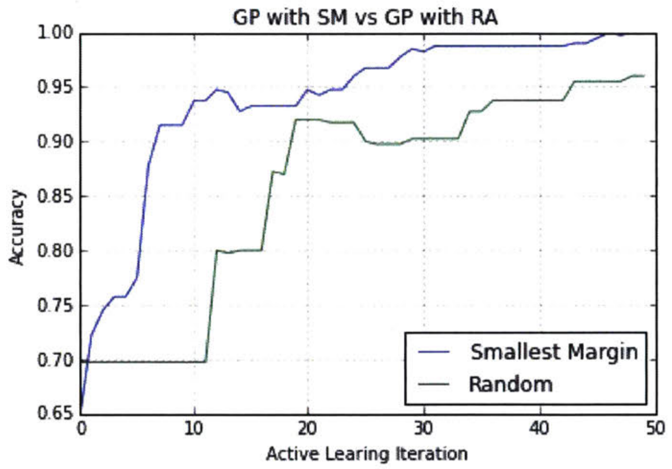


Figure 5-1: This graphic depicts the performance of area under the accuracy curve for an experimental run with Gaussian Process Classifiers where one is using smallest margin and the other is using "random".

Given these two bits of knowledge, we can know exactly how beneficial a query is for learning the ground truth and, if using the same type of model as the ground truth model, we know exactly what the weights have to be. Therefore, we created an evaluation metric to take advantage of this benefit which is the area under the accuracy curve and calculated as such:

$$Area\ under\ the\ Accuracy\ Curve = \sum_{n=1}^{N} Accuracy_n$$

Since accuracy alone is a static measure and does not consider the progression in accuracy improvements, we aggregate over active learning iterations to capture these changes that can differentiate one method from another. In Figure 5-1, we drew on two single experiments from the many active learning simulations: one with a Gaussian Process Classifier that uses smallest margin active learning and another that uses a Gaussian Process Classifier with random sampling. We can see that the Gaussian Process Classifier experiment that used the smallest margin active learning method has substantially more area under its accuracy curve relative to the Gaussian Process Classifier experiment that used the random sampling method which signifies better performance.

5.3 Machine Learning Model Selection

For machine learning model selection, we outline the process that we use to simulate many variations of active learning experiments for a chosen model in Algorithm 3.

Algorithm 3: Testing ML Models for Robustness

```
Input  : Max Iterations $I$ , Number Experiments $E$, Maximum Range values
         $Max_v$, Minimum Range values $Min_v$, Stepsize values $S_v$, Number of
         Variables $v$, Initial Number of Data Points $I_0$, Number of Queries $N_Q$
Output: mean and standard deviation of $C^E$
1  Pick an untrained model $f_R$ for robustness testing.
2  Pick an active learning method $AL$.
3  Initialize $C^E$ as an empty list.
4  for Ground Truth model $f_{GT}$ in Table 5.1 do
5      for $i = 0$ to $E$ do
6          $X_{all} \leftarrow$ Data_Generator($v$, $Max_v$, $Min_v$, $S_v$).
7          $X_{Query} \leftarrow$ randomly sample $I_0$ data points from $X_{all}$.
8          Initialize $X_{TRAIN}$, $Y_{TRAIN}$, $Accuracy_i$ as empty matrices.
9          for $j = 0$ to $I$ do
10             $Y_{Query} \leftarrow f_{GT}(X_{Query})$.
11             Append $X_{Query}$ to $X_{TRAIN}$ and $Y_{Query}$ to $Y_{TRAIN}$.
12             Train $f_R$ on $X_{TRAIN}$.
13             $\hat{y_R} \leftarrow f_R(X_{all})$.
14             $y_{GT} \leftarrow f_{GT}(X_{all})$.
15             $Acc \leftarrow \frac{1}{P}\sum_{n=1}^{P}\delta(y_{GT,n} == y_{\hat{R},n})$ where $P$ = length of $y_{GT}$
16             Append $Acc$ to $Accuracy_i$.
17             $X_{Query} \leftarrow$ Proposer( $f_R$, $X_{ALL}$, $AL$, $N_Q$)
18         end
19         Append $\sum_{n=1}^{I} Accuracy_{i,n}$ to $C^E$.
20     end
21 end
22 return $MEAN(C^E)$, $STD(C^E)$
```

To test the Gaussian Process Classifier and Neural Networks for robustness, we ran Algorithm 3. The inputs that we used for testing the machine learning model robustness are shown in Table 5.3.

Input Name	Value
Number Experiments	100
Number Iterations	50
N dimensions	2
Minimum Range values	[-100,-100]
Maximum Range values	[100,100]
Stepsizes values	[10,10]
Initial Number of Data Points	3
Number of Queries	1
Active Learning Method	Smallest Margin

Table 5.3: ML Model Robustness Test Inputs

The results from our experiments are shown in Table 5.5 and key findings are mentioned in Section 5.4.

Model	Area Under the Accuracy Curve	Standard Deviation
Neural Networks	47.50	2.60
Gaussian Process Classifier	46.61	1.37

Table 5.4: Results from Model Robustness Tests

Additionally, we provide a boxplot visualization in Figure 5-2 to show how area under the accuracy curve and the variance of the area differ.

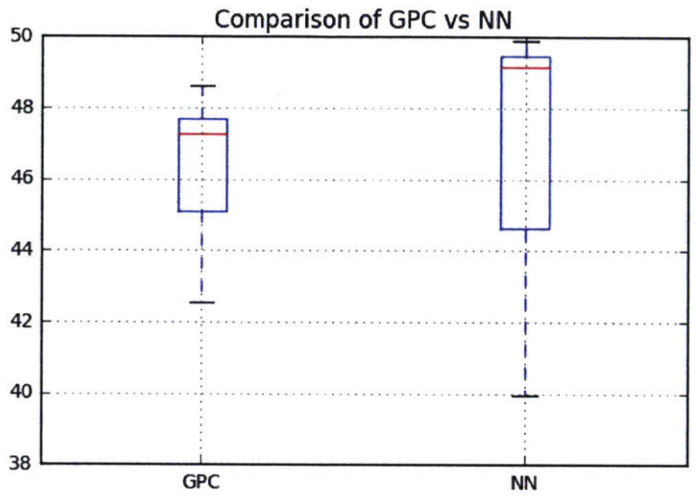


Figure 5-2: This graphic depicts the performance of area under the accuracy curve for Gaussian Process Classifiers compared to Neural Networks with one standard deviation bounds.

5.4 Active Learning Method Selection

For active learning method selection, we outline the process that we use to simulate many different variations of active learning experiments for a chosen method in Algorithm 4.

Algorithm 4: Testing Active Learning Methods for Robustness

```
Input  : Max Iterations $I$ , Number Experiments $E$, Maximum Range values
         $Max_v$, Minimum Range values $Min_v$, Stepsize values $S_v$, Number of
         Variables $v$, Initial Number of Data Points $I_0$, Number of Queries
         $N_Q$, Active Learning Method List $AL_{ALL}$
Output: vector of means and standard deviations for each method in $AL_{ALL}$.
1  Pick an untrained model $f_R$.
2  Initialize $C_{MEAN}$ and $C_{STD}$ as empty lists.
3  for $AL$ in $AL_{ALL}$ do
4      Initialize $C^E_{AL}$ as an empty list.
5      for Ground Truth model $f_{GT}$ in Table 5.1 do
6          for $i = 0$ to $E$ do
7              $X_{all} \leftarrow$ Data_Generator($v$, $Max_v$, $Min_v$, $S_v$).
8              $X_{Query} \leftarrow$ randomly sample $I_0$ data points from $X_{all}$.
9              Initialize $X_{TRAIN}$, $Y_{TRAIN}$, $Accuracy_i$ as empty matrices.
10             for $j = 0$ to $I$ do
11                 $Y_{Query} \leftarrow f_{GT}(X_{Query})$.
12                 Append $X_{Query}$ to $X_{TRAIN}$ and $Y_{Query}$ to $Y_{TRAIN}$.
13                 Train $f_R$ on $X_{TRAIN}$.
14                 $\hat{y_R} \leftarrow f_R(X_{all})$.
15                 $y_{GT} \leftarrow f_{GT}(X_{all})$.
16                 $Acc \leftarrow \frac{1}{P}\sum_{n=1}^{P}\delta(y_{GT,n} == \hat{y_{R,n}})$ where $P$ = length of $y_{GT}$
17                 Append $Acc$ to $Accuracy_i$.
18                 $X_{Query} \leftarrow$ Proposer( $f_R$, $X_{ALL}$, $AL$, $N_Q$)
19             end
20             Append $\sum_{n=1}^{I} Accuracy_{i,n}$ to $C^E_{AL}$.
21         end
22     end
23     Append $MEAN(C^E_{AL})$ to $C_{MEAN}$.
24     Append $STD(C^E_{AL})$ to $C_{STD}$.
25 end
26 return $C_{MEAN}$, $C_{STD}$
```

To test the active learning strategies for robustness, we ran Algorithm 4. The inputs that we used for testing each active learning strategy's robustness are shown in Table 5.5.

Input Name	Value
Number Experiments	100
Number Iterations	50
N dimensions	2
Minimum Range values	[-100,-100]
Maximum Range values	[100,100]
Stepsizes values	[10,10]
Initial Number of Data Points	3
Number of Queries	1
Active Learning Method List	[Smallest Margin, Entropy, Random]

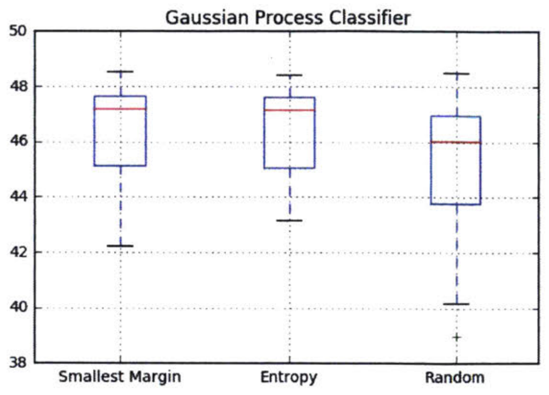
Table 5.5: Active Learning Robustness Test Inputs

The results from our experiments are shown in Table 5.6 and key findings are mentioned in Section 5.5.

Strategy	$Area_{GP}$	Std_{GP}	$Area_{NN}$	Std_{NN}
Smallest Margin	**46.5470**	**1.2976**	**47.5146**	2.5976
Entropy	46.5271	1.3364	47.3719	2.5857
Random	45.3844	1.6100	45.8832	**2.4247**

Table 5.6: Results for Active Learning Robustness Testing

Once again, we provide a boxplot visualization in Figure 5-3 to show how the area under the accuracy curve differs from the standard deviation.



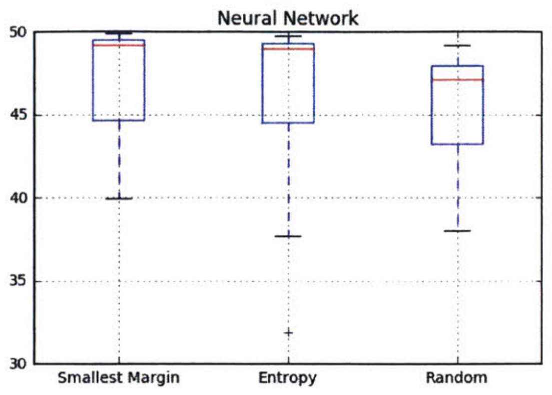


Figure 5-3: This graphic displays the average area under the accuracy curve for the Gaussian Process Classifier and Neural Networks, the corresponding active learning methods, and the one standard deviation above up to 50.0 and below.

5.5 Key Findings

To reiterate, the objectives of these experiments were to answer the following questions:

- **What is the most robust machine learning model?**
- **Does active learning help in this thesis?**
- **If more than one active learning method does help, which one is the best?**

As a result of running these experiments, we derived the following key findings:

1. The Gaussian Process Classifier was the more robust nonlinear model for classification. The standard deviation of the area under the accuracy curve for the Gaussian Process Classifier was 53% of the Neural Networks' standard deviation.

2. We found that active learning does consistently help with Gaussian Process Classifiers but there are a couple nuances with respect to using them with neural networks. Neural networks had the least variation in performance with the "random" method but better average area under the accuracy curve for

the active learning strategies. We see that active learning actually biases the neural network into creating non-robust boundaries which is consistent with [2]. Therefore, in the case of neural networks, there is a potential trade-off when using active learning since accuracy gains will be less consistent.

3. From the active learning experiment, we found that smallest margin was the most robust active learning method for Gaussian Process Classifiers. This makes sense since our evaluation metric is area under the accuracy curve and smallest margin is better known for improving classification accuracy specifically compared to entropy. [16] However, for neural networks, smallest margin was actually the least robust active learning method. This returns us to the problem of lacking a base of data prior to using active learning.

Chapter 6

Conclusion

6.1 Key Findings

Overall, we found that COAL was successful in achieving our objectives of achieving robustness and accuracy gains superior relative to passive learning.

COAL can capture a wide variety of unknown nonlinear relationships. In our robustness experiments, we train multiple nonlinear oracle models to determine the robustness of models and active learning strategies. Despite the nonlinear nature of these models, the active learning methods were able to adeptly identify the most informative data points which made it possible for the machine learning models to converge to the oracle model's accuracy.

COAL implements active learning strategies that consistently outperform passive learning. In our experiments where we determine the effectiveness of each active learning method, we found that active learning methods consistently outperform passive learning methods with higher cumulative accuracy and lower standard deviation in performance.

6.2 Contributions

In this thesis, we:

1. Designed COAL, a system that allows users to leverage machine learning models

and active learning methods to query for informative data points.

2. Introduced the concept of synthesizing various nonlinear oracle models in order to test the robustness and ability of active learning strategies and models.

3. Demonstrated that, based on a variety of hidden underlying oracle functions, the Gaussian process classifier was a highly robust model for integration with active learning strategies.

4. Demonstrated that, based on a variety of hidden underlying oracle functions, the smallest margin active learning strategy was the most robust strategy for improving Gaussian Process Classifier accuracy but had a tendency to bias Neural Network models.

5. Demonstrated that regardless of the active learning strategy chosen, users should highly consider implementing active learning strategies in their data gathering processes to enjoy the almost consistent label savings that come with its application.

6. Created an evaluation metric that is industry focused and will allow users to identify the quality of their combination of machine learning model and active learning strategy.

6.3 Future Work

In future work, there are multiple avenues that we could pursue in order to expand on the current capabilities of COAL. The following three areas are where we believe research will further add to the conviction of our system in COAL and improve the robustness and accuracy of our approach.

1. **Considering More Models**: While we looked into how Gaussian process classifiers and neural networks behaved relative to the active learning strategies we used, we would like to further confirm our belief that Gaussian process classifier is the most robust model to be used in these active learning scenarios. Other

potential models include support vector machines and quadratic discriminant analysis which are also models in machine learning literature known for adeptly capturing nonlinear relationships.

2. **Considering More Active Learning Strategies**: Implementing and using other active learning strategies was another area of interest that we wish to pursue in future research. There are a variety of other methods for different application scenarios. Given our current method and for single query processes, expected model change [18] and expected error reduction [12] are two viable strategies for COAL's use case. Another area that we are also interested in expanding into with COAL is the use of formal batch mode active learning strategies. In cases where multiple queries are to be requested per iteration, batch mode active learning takes in additional considerations that single query strategies often do not in order to provide more robust baskets of data points to query.

3. **Considering Costs More Specifically**: Given that COAL is a system geared towards industry use, we found that often times, industry researchers are faced with economic constraints. As a result, perhaps one of the most promising future paths for our research is to integrate the costs for each variable. If we assume that costs are linear as one uses more or less of a given variable, then we can easily solve for the cheapest product solution via a simple linear program. From here, COAL would be able to focus on an even smaller subsection of the variable space than the pre-specified constraints which could result in faster and more optimal results for industry users.

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