Experiment Based Crafting and Analyzing of Machine Learning Solutions

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Chapter 1

Introduction

The last decade has seen unprecedented growth in the deployment of Machine Learning (ML) based solutions broadly influencing many aspects of our lives.\textsuperscript{1} Significant progress has been made in machine learning tasks such as image recognition, language translation, and tasks related to self-driving cars, to name a few. With such prospects of potential success, the industry is attempting to apply ML to a variety of use cases at an unprecedented rate, including for crime prevention, medicine, IT and cloud analysis, cyberspace security, intelligent chatbots, and various ”AI agents” that provide services in various domains.

ML based solutions are composed of ML models and regular software to achieve some common goal, e.g., making the driving decisions of the self-driving car. But what are ML models? ML models can be thought of as regular programs that were produced by automatically searching over some predefined set of possible programs. The search is guided by examples of the desired program behavior. We usually refer to the examples as the training data or simply as data. Thus, just as we teach young children by example, in this case we have given the machine examples from which it learned the correct behavior; hence, the name machine learning.

ML models are statistical by design. We do not expect to find an ML model that is always correct. In fact, we are unlikely to know whether the space of possible models that we search in contains such a perfect model, and even if it does it may be too difficult to find. Instead we settle for the model being correct most of the time. In addition, we require that a successful model will be correct most of the time on unseen data of the same type as the data is was trained on. We call this desired trait generalization. Thus, a bug in an ML model usually cannot be determined from the individual response of the model to a single data point; rather, it is determined by the aggregated behavior of the ML model on many examples. As a result, an ML solution composed of several ML models and regular software can only be successfully crafted if it is validated by statistical experiments. It also means that the required behavior of an ML solution can only be defined as an aggregate of its behavior on individual data points. In the case of a self-driving car, for example, we can specify that the desired average number of wrongly recognized cars is no more than 5%.

We thus emphasize the definition of quantitative measures that reflect the desired behavior of the ML-based system; a system composed of ML models and regular software. An example of such a measure is the average number of service calls a chatbot is routing to a human agent. We refer to such measures as requirement measures. We focus on analyzing the requirement measures that capture the desired behavior of the system. We do so

\textsuperscript{1}See CNN 2019 article for more details - https://edition.cnn.com/2019/12/21/tech/artificial-intelligence-decade/index.html
using an appropriately designed statistical experiment that estimates the expected average and variance of those measures. A good experiment will provide accurate estimates of the requirement measures when the ML based system is deployed. This practice tackles the challenge of crafting a robust ML solution.

Creating a good set of training examples for a given requirement is challenging too. The data may be lacking criteria without which the desired model cannot make correct decisions. We might have too few examples, or examples that are not representative of the type and distribution of data that the system will encounter when the model is applied. Finally, in order to guide the learning, the data needs to include the "correct answer" as well as indication that it is indeed correct. Such indication is typically provided by labeled data, in which case the problem is a supervised learning problem. However, it often happens that an organization holds a representative set of examples that is readily available but are not labeled.

As mentioned above, this book aims to address the challenges of crafting robust ML solutions that meet their design requirements and hence can be confidently deployed. We focus on an experimental approach to the crafting of ML solutions. This approach can be thought of as the ML equivalent of the test-first approach applied with regular software. To emphasize this similarity, we name our approach experiment-first. The focus of this approach is on crafting, validating, and continually monitoring ML-based solutions via a series of carefully designed experiments at different levels of abstraction. The book is self-contained and addresses the mathematical and statistical techniques needed to apply the experiment-first approach. It contains numerous practical programming as well as theoretical exercises and their solutions. Exercises are an integral part of the text and are designed to facilitate understanding of the ideas, concepts and methods introduced. The book does not address low-level engineering concerns such as the need to be able to automatically re-train ML models, save the data that was used for training, and trace it to the model that was obtained from the training. These topics are well covered in the literature, e.g., tutorial on MLops.

The main target audience of this book is data scientists who craft ML-based solutions, architects who define what the solutions need to do, and testers who need to validate that the system actually works and meets its specifications. The book also attempts to bridge communication gaps between the stakeholders involved in the development of ML-based solutions. The experiment-first approach introduced in this book facilitates an end-to-end, unambiguous, quantitative definition of the steps to be taken in the development of an ML-based system. Our approach details the activities performed, and the artifacts consumed and generated, throughout the development and deployment of the solution. The book introduces the statistical experiment and its results as the language by which the stakeholders communicate effectively to craft the ML-based solution.

ML-based solutions raise several concerns that are out of the scope of this book. As a ML model learns from existing data, its ability to make inferences may be affected data bias. For example, gender bias in the ML model may result when learning from historical data that includes that bias. In addition, private data may be used for learning, and data can be manipulated by attackers to change the learning results. There might also be legal concerns that would require an explanation of the rationale behind a decision made by the ML model. Much research addresses these concerns, with the goal of enabling and facilitating the deployment of ML models. See [14].

The above concerns are sometimes collectively referred to as trust concerns. This book does not focus on trust concerns. Instead, when following the experiment-first methodol-
ogy, the appropriate set of trust concerns that are relevant the ML solution at hand will
naturally surface as the system requirements are defined. This will then lead to the design
of experiments that address these trust concerns. At that point, it is advisable to apply
state-of-the-art techniques related to trust and model readability[16].

Experiments are best designed by following the scientific method, which includes the
definition of a problem, the formulation of a quantitative conjecture, and the design and
implementation of an experiment that validates or rejects the conjecture. For example,
a problem could consist of finding the speed at which a ball will touch the ground when
dropped from a high tower. The conjecture is that the speed is proportional to the time,
and the experiment involves dropping balls from towers of different heights and measuring
how long it takes them to hit the ground.

This book is organized as follows. In Chapter 2 we paint in broad strokes the scientific
method and highlight its relation to ML system development and validation. As mentioned
in the previous paragraph, following the scientific method includes defining a problem,
making a conjecture that may solve it, and then designing and implementing an experiment
to check and validate the conjecture. When crafting an ML-based solution, the problem is
defined by the system requirements. The standard conjecture entails generalization, namely,
that the system will behave as required on new inputs not seen before. We then address
specifics of how to formulate a generalization conjecture and how to craft the appropriate
experiment to validate it and analyze the results in the event that the conjecture was wrong.
We also highlight the way i which the results of the experiments influence system design
and contribute to the continual monitoring and validation of the system throughout its
life-cycle.

Then, Chapter 3 details practical aspects of the experiment-first methodology. They are
described as a set of pitfalls and best practices that are designed to quickly reduce the risk
of the development of the ML based system and help address the most important concerns
first. Practices proposed in Chapter 3 should allow stakeholders to better validate, from
day one, the potential for successful generalization given the business requirements and
data. They should additionally assist in estimating possible improvements in the chances
of success in creating a ML based system via optimal usage of information extracted from
the data and application of the most suitable ML techniques to the problem at hand.

When analyzing ML models the focus is sometimes on generic measures, e.g., the ac-
ccuracy of the model. In contrast, an ML-based solution has unique, specific requirements.
For example, a chatbot may be required to send no more than 10% of the conversations
to a human agent. In addition, specific requirements are frequently realized through the
interaction of more than one ML model as well as regular software. Chapter 4 discusses the
composition of ML software and regular software in a unified ML-based system, and how
such composition impacts system validation.

The next two chapters on ML testing (Chapter 5) and on drift (Chapter 6) address
the system correctness concern at different phases of the project. The ML testing chapter
focuses on checking system correctness before it is deployed, while the chapter on drift
detection analyzes whether the system operates correctly once it is deployed.

As the basic conjecture made about ML-based system correctness entails the general-
ization of some measure, e.g., the volume of service calls that were sent to a human agent
in a chatbot scenario, the experiments that are done at testing time should project that the
desired behavior will manifest once the system is deployed. Due to the stochastic nature
of ML-based systems, the validation typically includes a stability claim. For example, on
average 5% of the service calls are diverted to a human agent but it is unlikely that more
than 10% of the calls are to be diverted.

As data changes over time the system might fail to meet the desired behavior once it is in operation, even if it was well built and tested. For example, in the chatbot scenario, changes in the type of service calls might result in much more than 10% of the calls being diverted to a human agent. To handle this, drift detection is required. This topic is covered in Chapter 6.

Once the expected system behavior is established, we can define an optimal business process. In the chatbot example, once we know that up to 10% of the service calls are diverted to a human agent, we can plan the size of the customer service team that will provide proper response to the diverted calls. The integration of ML-based system behavior with the business process is discussed in Chapter 7. Finally, in Chapter 8, we present an industrial example to demonstrate the implementation of principles of the experiment-first methodology in practice.

Solutions to exercises that appear across the book, code samples and mathematical background are found in the appendix.
The greatest risk of a ML project is whether or not we can learn, i.e., build good ML models from data. Typically, training data will also serve as input to the ML solution once it is deployed. The fundamental assumption of ML theory is that the data used for learning is representative of the data that will be encountered once the ML solution is deployed. Thus, the fundamental requirement from a good learning system is generalization - the ability to create rules that will work on data input of the same sort. For example, a ML model that was trained to identify a human face on data that includes all types of animal and human faces is not expected to work well when presented with a picture of a car. As typical in software engineering, the biggest risk of a project should be addressed first. Thus, we should first address the question of whether, given the available data and the business requirement, we can successfully learn? To address this concern, we design experiments whose results indicate how we can learn, if at all, the type of decomposition to components or architecture the system should have, and the next development iteration and experiments.

**Example 1.** Our ML solution needs to determine the risk level an investor desires and different major expenses she is about to encounter, such as paying the kids’ college tuition, buying a new house or going on annual vacations. The available data is the investor’s personal profile, past investment history, and assets inventory. There are many possible architectures. We can create one monolithic ML model. In contrast, and on the other end of the spectrum, we can build a ML model that tries to predict the desired investment risk level and a model for each possible major investment, e.g., buying a house. We can also have a single model for all of the expenses. Finally, the models output that predict the expense types can be used as input or features in the learning of the risk level model. Chapter 3.5 will provide insights into the tradeoff involved in choosing the right architecture, but the ultimate check is an experiment in which the different approaches are compared and the best choice is determined.

**Exercise 2.0.1.** A self-driving car is trained using data on traffic in Tokyo. The manufacturer claims that the car can drive in large European cities as they are similar to Tokyo. Form an opinion about the claim and discuss relevant factors that you think impact the self-driving car’s performance. What experiment might validate the manufacturer’s claim?

It is useful to draw an analogy with the Test First software development process. In Test First, a functional test is written before the code is implemented. The test formally
defines what the system is required to do. The code that is implementing the functionality captured by the test is then implemented. Next, the test is executed against the code. If the test passes, then the code is OK. The test is added to a set of passing tests that accumulate and serve as a functional test suite of the system being developed. At every development stage, all tests in the test suite must pass before the next test is designed.

In the case of a ML solution, an experiment is defined instead of a test. The experiment results are used to determine whether the system meets the requirements, but with two major differences: (1) the experiment result is a statistic, e.g., an average, and not a success or pass binary result; and (2) the experiment result may help us choose among design alternatives.

Exercise 2.0.2. Given a number, $x$, a function returns $x^2$ most of the time, i.e., in $p$ percentage of the cases. Write a test that finds the percentage $p$. How is that different from a test that checks that a deterministic function correctly evaluates $x^2$?

Click here for a Solution. TBC - the solution has foo(3). Any other number could have been used. Explain.

Exercise 2.0.3. Test First goes hand in hand with automation; we require that the test suite can be run and its pass or failed results determined programmatically. What is the analogous requirement in the case of an experiment-based approach to ML development?

We conclude that a good ML project consists of a series of statistical experiments. The results of each experiment reduce the risk of the project and help determine its architecture. It is similar to a sail boat that depends on the direction of the wind - the data in our case is the wind. This approach, which we will call Experiment First, focuses on simultaneously considering the data and the business goal from day one. We next take a deeper look at the design and analysis of statistical experiments and how they relate to the practice of Experiment First.

TODO: add a general mapping of the scientific approach to AI analysis to setup the stage for the more detailed discussion in latter chapters in second part of the book.

2.1 The scientific method

The scientific method includes the consideration of a problem, the formulating of a conjecture, the design of an experiment that can validate or refute the conjecture, and then the analysis of the results of the experiments. Insights from the analysis of the experiments lead to the formulation of new conjectures and new experiments, and the process repeats itself.

The scientific method is general. It applies to problems such as finding a cure for a disease, discovering the laws that govern the movements of bodies, or determining whether a production line is reliable. The experiments used to validate the conjectures we have made with regard to such problems are designed using statistics as an underlying technique. We will explore the design and analysis of statistical experiments with a focus on ML, but first we will consider a simple example of the scientific method from mechanics.

Example 1. The problem is to determine the rule that governs "free fall" on Earth and the Moon. We drop a small metal ball from a height of 2 meters and use a camera to determine where the ball is after 1 ms, 2 ms, etc. We repeat the same experiment on Earth and on the Moon. Analyzing the results, we see that the location at time $t$, $x(t)$, is given by a formula of the form $x(t) = At^2$, where $A$ is a constant that has different values on the
Moon and on Earth. We are happy and declare victory - in determining the rule of "free fall".

**Exercise 2.1.1.** Can you suggest why the above conclusion is not correct. **Clue** - think about letting other objects fall.

It turns out that designing good experiments is tricky in that it requires domain knowledge: we need to think about the factors that influence the results of the experiment, which is hard to do if we lack that knowledge. In the experiment above, factors such as wind or the nature of the object being dropped, e.g., a feather instead of a metal ball, are applicable to the Earth but not to the Moon. Similarly, domain knowledge is key to the successful design of ML solutions. This is common knowledge, often expressed through feature engineering, among other things. Feature engineering is the practice of designing the features extract from the raw data that will be used in the learning process. What is less obvious is that domain knowledge is also the key to the analysis and validation of ML solutions. The Experiment First approach emphasizes this point. In this approach, domain knowledge is embedded in the validation process through careful design of the experiments and identification of the factors that govern them. We next consider the relation between the scientific method and the ML solution development process.

### 2.2 Mapping the scientific method to ML development

As discussed in the previous section, following the scientific method includes defining a problem, coming up with a conjecture and the design, implementation and analysis of an experiment that confirms or rejects the conjecture. In the case of ML embedded systems the problem is expressed in the form of a business requirement. For example, the bank would like to develop a system that determines if to give a loan to a customer or not. The conjecture may be that the personal and past data on the customer financial transactions is enough to create a ML that determines if the bank can make a profit from giving the loan. The experiment will constitute determining the performance of the ML on a new and representative set of customers. In other words, checking if the ML model was able to determine correctly from the personal and financial transaction data of a fresh set of bank customers that the model has never seen before if the bank will profit from giving the loan or not.

Key points in the design and analysis of the experiment include translating the business objective to quantitative measures that can be measured in the experiment, determining the factors that are impacting the experiment, insuring coverage of these factors, and statistically analyze the experiment outcomes to reliably deduce results from the outcomes. Error and randomness should be taken care of when analyzing and interpreting the results. The last point is illustrated by the next thought exercises.

**Exercise 2.2.1.** We consider the tossing of two coins 100 times. This is done for two coins. The first coin turns head 80 times and the second coin turns head 85 times. Is the second coin more likely to turn head than the first one? Discuss why it may be the case that it is not. How would you go about increasing your confidence that the coins have a different chance of turning head?

**Exercise 2.2.2.** The bank also has data on whether or not its customers paid previous loans. Using that data customers who previously paid on time are labeled as customers that
"can be given a loan" but if they did not pay on time they are labeled as "can not be given a loan". Only using data available before the loan was given, two ML models that predict if the customer can be given a loan are developed. Next the percentage of correct answers the models gave is calculated on a fresh set of customers that were given a loan. One model predicts correctly 80 percent of the time and the other 85 percent of the time. Which model is better and how is the answer to the question related to the previous question with the coin tossing?

It is important to note when analyzing ML embedded systems that randomness is ingrained in the solution. If we use the two models developed for loan prediction in different time windows we expect percentage of the correct answers to change. We are thus interested in whether or not most of time it is likely that the percentage of correct prediction of one model is going to be larger than the percentage of the correct prediction of the other model. This is a statistical question and requires statistical techniques we will develop in chapter 5.

Two other points are interesting to note when considering the bank loan example. The translation of the business requirement to a quantitative measure is a non trivial part of the system definition as well as the experiment definition. In our case, a customer could be late, but not too much, and still the bank may make a profit on the loan. Thus, other more refined labels could be defined. In addition, there are customers that were never given a loan. Maybe such customers are of different "type"? Maybe our prediction will not work well on customers that were never given a loan? Consider the following thought exercise.

Exercise 2.2.3. Can you suggest a new experiment that will help distinguish if the models have different performance on customers that were never given loans before? What would be a conjecture in this case?

We could distinguish between customers that were given a loan only once and customers that were given a loan more than once. We can then take the label for loan payments for each loan the bank gave to the customer separately. We can thus have a model for customers that were given the loan for the first time and design a second experiment that determines if the model work well on such customers. In fact we have identified a factor that governs the experiments, namely, whether or not customers are given a loan for the first time and an implicit requirement - the model should preform well on customers that are given a loan for the first time as well as on customer that were previously given a loan. Such a factor identification leads to an architecture question - should we have two models one for customers that were never given a loan before and one for customer that were?

Exercise 2.2.4. How would you determine which architecture option to take?

We have seen how business requirements are translated into quantitative ML embedded systems performance requirements on fresh data. We also seen how an experiment designed to validate initial models lead to the identification of factors governing the experiment, the identification of not yet articulated business requirements and the design of additional tests to validate the evolving ML embedded solution performance and determine its architecture. Next, we will discuss each stage of the scientific method in the context of ML in more details.

A comment on randomness is in order. When we say that we choose a fresh sample, we mean that we randomly choose a new set of customers. If the choice is skewed, for example with more customers that were previously given a loan, then the percentage we
obtain may be skewed and not reflect the real behavior of the system. The important point is that randomness will take care of factors that impact performance even if we have not yet identified them - a fundamental principle of statistical experiment design that applies to the crafting and analysis of ML solutions. We will revisit this point in various ways throughout this book.

2.3 Conjectures

We next continue in the discussion of the relation between the scientific method and the development of a ML embedded system and recall that the scientific method includes the following steps - problem definition, conjecture formulation and experiment design. The problem is defined by the system requirements and the conjecture is driven from them. Deriving the conjecture includes the translation of the system requirements to a quantitative measure and the identification of factors that govern the quantitative measure and desired performance expressed using this measure. Typically, the ML conjecture is that independent of the governing factors the quantitative measure desired performance can be learned. Learned here means that the ML embedded system will perform according to the desired level as measured by the performance measure on new data that was never used in the training of the ML models embedded the system.

Interestingly the step of quantifying the system requirements and the factors that govern them help identify system requirements that are not a good candidate to be implemented as a ML embedded systems. Generally speaking systems could be too complex or too simple to be good candidates for a ML emended implementation. If a close form of the relation between the governing factors and the desired performance can be expressed and only the optimal parameters that define the relation obtained, the desired system is a too simple to be a good candidate for a ML embedded implementation. The example of the law of mechanics that were given above is a good example of such a system. On the other hand, if the governing factors are hard to identify and it is not clear of what type the relation that implements the system is the system is too complex and will probably not be a good candidate for a ML embedded system implementation. An example of that is a long term accurate weather prediction systems. There is a sweet spot in between of the two extreme which serves as a good candidate for a ML embedded solution which we discuss next.

A good ML solution candidate will at least meet the following criterion.

1. We are able to quantify the business requirements.
2. The factors that govern the business requirements can be identified.
3. We identify a search space in which we can search for a good solution automatically. This is sometimes referred to as the learning phase and the search space is referred to as a model (e.g., a regression, a neural network with some specific architecture or a decision tree).

The last requirement is many times met implicitly by choosing a ML learning method that previously worked well in some domain, e.g, convolution neural network (CNN) for anomaly detection. Making it an explicit step increases the chance of successful learning. In addition, autoML [??] can help automate this step. The following exercise is designed to help clarify the concepts of a model and model choice. It requires experience in the use of ML libraries and training. If such experience is not available it is recommended that the
reader will go through some tutorial on linear regression using Python before attempting the exercise.

Exercise 2.3.1. A parabola, i.e., \( f(x) = ax^2 + bx + c \), is given. 100 samples \( D = \{(x_1, f(x_1)), \ldots, (x_n, f(x_n))\} \) are obtained by randomly choosing \( x_1 \ldots x_n \) and then calculating \( f(x_1), \ldots, f(x_n) \). \( D \) is used to train a linear regression model of the form \( g(x) = dx + e \).

1. Do you expect the results to be good? Explain your reasoning.

2. Implement the above scenario using standard learning libraries. Validate whether or not the obtained linear regression was good.

3. Provide a graph view that presents \( f() \) and the linear model obtained by applying the regression on \( D \). How does that help understand the performance of the linear model?

4. Is there any pair of parameters \( d \) and \( e \) of \( g() = dx + e \) that will work well?

5. Use the following feature engineering. Define \( D' = \{(x_1, x^2_1, f(x_1)), \ldots, (x_n, x^2_n, f(x_n))\} \). Apply linear regression on the new data set. Did the results improve? Can you explain why?

6. What will happen if you add some noise to the data? Concretely, randomly choose some \( \text{noise}_i \) from the standard normal distribution, \( N(0,1) \), \( n \) times and change the data to \( D = \{(x_1, f(x_1) + \text{noise}_1), \ldots, (x_n, f(x_n) + \text{noise}_n)\} \). How would your answers change given the new data set?

7. Does the size of the dataset \( D \) matters? if so, how?

Click here for Colab Solution.

TBC - explain how the parabola example is related to the model concept.

TBC

2.4 Experimental design

We have discussed derivation of a quantitative performance measures from business requirements and the identification of factors that impact the performance measure. In the language of statistical experiments a performance measure is referred to as the dependent variable and the factors that impacts the performance measure are referred to as the independent variables. Our implicit conjecture is that regardless of the value of the dependent variables the performance of the ML embedded system on new unseen data will meet the require performance level as defined on the performance measure. For example, the performance level may require that the average percentage of wrongly predicting that the bank will make a profit when giving a loan to a customer is 10%. In addition, its variance is required to be small.

In order to conduct the experiment, we will typically collect a set of input data and apply the ML based system on the data to obtain an estimate on the performance of the dependent variable. We would like the identified independent variables to appear in the data. In reality one can not expect to identify all of the independent variables. We thus expect to have some latent variables, possibly with their value appearing in the data, that impact the dependent variable we are estimating. Unfortunately, the dependent variables may not even be in the data.
Denote the dependent variable by $Y$, the identified independent variables by $X_i$ and the unidentified independent variables by $X_j$. As we collect our data for our experiment we need to take into account the following.

- Make the data records as comprehensive as possible. Include available features in the data record, e.g., age of the customer, if available even if it is not required as input to the ML based system and it is not identified as an independent variable. This will allow for further analysis aimed at discovering the latent variables $X_j$.

- Avoid bias. Avoid collecting the data in a way that consistently favour some data record features. One of the ways to mitigate the issue of latent variables is to randomly sample the experiment data. If this is not done fundamental assumptions underlying the theory and practice of ML are broken. In addition, by randomly sampling the data the impact of latent variables $X_j$ appearing in the data is amortised and we can still estimate the behaviour of the dependent variable $Y$ although we did not identify the latent variable.

- Choose whether or not to stratify values of dependent variables. For example, we are given a medical system that decides if a new drug’s side effect should be reported to the government based on medical reports. An independent variable is the type of the report. There are two types of medical reports - hand written reports and digital reports. We may be interested in the system performance when the report type, $X$ is $X = \text{handWriten}$ and when $X = \text{digital}$. We will thus have two different predictions, one for each value of the independent variable $X$. This is called stratification. On the other hand, we may choose not to stratify the independent variable. That brings us back to the randomization guideline. We need to take extra care that the variable is not biased. For example, if our sampled data mostly have digital reports we can not expect to draw conclusions about the performance of the ML based system on hand written reports. When do we stratify? When we want the analysis and predication at that level of details to clarify if the system really meets the business requirement. The business requirement in our case is that the the system will work well on both values of the variable $X$ (hand written and digital). Note the obvious dilemma. If we stratify all possible values of the independent variable $X$, we will get a combinatorial explosion of stratified values. we will revisit this issue later in the chapter.

The following exercise is designed to demonstrate the concepts of randomness and stratification.

**Exercise 2.4.1.** The unknown relation the system had to learn is $f(X, Y, Z) = X + Y^2 - Z^3$. $X$ and $Y$ take values in $\{-1, 1\}$ while $Z$ is a number, $Z \in \mathbb{R}$. We identified the independent variable $X$. Data was sampled as follows. $X$ was set to -1, $Y$ was randomly chosen. $Z$ was randomly chosen from a normal distribution with average 5 and variance 1.

1. How is the data biased?
2. Suggest a correction to the sampling method
3. How would you conduct a stratification on $X$?
4. What are the hidden variables?
5. Assume that the system was implemented as \( g(X, Y, Z) = Z + Y^2 - Z^2 \). Implement an experiment that analyze the performance of this system and suggest ways to identify that \( Z \) is a dependent variable.

The following exercise is designed to shade light on sampling challenges used to collect the data.

**Exercise 2.4.2.** The ML systems attempts to determine if a child will graduate from school. Two independent variables are considered, namely, the child’s neighbourhood and the size of the child’s family. It is desired that the ML system will have the same level of prediction regardless of the values of the independent variables and we are collecting data to measure and determine if this is indeed the case (the experiment). Three sampling methods are considered as follows.

1. Randomly choose a child
2. Randomly choose the family size, then randomly choose a family of the chosen size, then randomly choose a child in the family that is attending school
3. Randomly choose a neighbourhood, then randomly choose a family that lived in the neighbourhood in the last 5 years and then randomly choose a child in that family

Can you identify bias introduced by the sampling techniques above? Assume the first technique produced a sample of 100 children and none comes from a family of more than 6 children. Can you still estimate the performance of the ML system? What would you suspect if no child from a family of one child was chosen in the sample?
Chapter 3

Pitfalls and Best Practices for the Machine Learning Designer and Tester

3.1 Overview

We are in the middle of the AI and data revolution. Companies are attempting to utilize data and realize business value. "Data insight" is an old-fashioned application of AI that does not recommend actions. However, businesses today want to trust AI in their decision making with and even without a human in the loop. This requires the creation of a business-grade reliable and trustable ML solution (or AI-infused solutions).

There are many good resources on ML technology as well as good courses on theory and algorithms. We are not attempting in this paper to fill that need; if we were, we would be presenting Yet Another Machine Learning Machine or YAMLM. Instead we are trying to highlight the best mindset that increases the chance that an ML project will succeed.

3.2 From day one determine if the data is relevant for the business objective

Deciding which business objective to implement depends on the data. The happy marriage of business requirements with relevant data is the determining factor in creating a high quality AI-infused system. It’s a waste of time to discuss the solution in isolation from the data and without directly inspecting and analyzing it to determine whether the business goal may be achieved. However, it may be useless to learn whatever is possible to learn from the data as such learning, even if successful, may not serve any useful business goal.

Following items should be added/integrated TBC:

- Data may or may not include significant signal supporting the business objective. For example, classification of software defects ODC (Orthogonal Defect Classification) vs. custom classification

- Data may have a signal that is ‘too strong’ Ex. It is always the case that a defect opened by a manager is of highest importance. No sense in learning this. Use a rule instead
• Explicitly measure business value; Don’t confuse ML metrics with business value.
• Explicitly measure business value - Don’t confuse ML metrics with business value
• Customize off-the-shelf ML measurements for experiments

3.3 Think science and experiments

AI-infused solutions are heavily dependent on data and are statistically correct by nature: they are by definition sometimes correct and sometimes incorrect. It’s the nature of the beast. Business-grade AI-infused solutions need to control the statistical error. Experimental design approaches should thus be introduced and analyzed. These experiments are equated with ML learning iterations. This will be further explained here. To reduce the main risk of AI-infused systems development, frequent experimentation is desirable and architecture should be driven by the experimental results. Consider a sailing ship attempting to reach point B from point A. The wind is not going from B to A and needs to be harnessed for the boat to reach its destination. In our case, the wind is the data and the sailing ship is the AI-infused system under development and the harnessing process is realized through experiments.

TBC:
• Explain the scientific method
• Explain design of statistical experiments
• Map statistical experiments to machine learning

3.4 Data must be of valuable volume; When not to use learning

Systems scale in complexity from the ones for which we cannot even list the factors that control them to the ones for which we can easily write their equations, e.g., a physical body that accelerates under a constant force. In such a case use rules; ML may be overkill. An intermediate situation is where the equation is known but a few constants should be empirically calculated, e.g., system performance tuning. Maybe a few cycles of experiments will do in such a case. Yet another intermediary case where ML shines is when only a general form is known (a model). We need to think of the choice of a ML technique as a choice of such a model. For example, a neural network is a model with a graph of thousands of neurons, where the connecting edges are associated with weights. Together the set of all weights is our model, and we are tasked with finding the best set of weights.

Even if we decided to apply learning, sufficient data is required to succeed. A rule of thumb for data sufficiency is that the size of the training data should be an order of magnitude bigger, e.g., at least 10x, than the number of features. If a classification task is attempted, the number of examples per label should be at least 30.

TBC:
• is the training data representative of the deployment data?
• Remember that you also need data for testing. When training – development set –
  used multiple times. When testing – test set – you cannot use it to change your model!
  If you do, you will need more data for testing.

• Remember labels. You cannot learn labels that are not in the training set. Need
to understand and control labeling mistake rate (see Estimate the probability of a
labeling mistake).

• Is data adequate for learning? A hybrid approach.

3.5 Use all relevant data and information: Do NOT ignore structure

When designing an AI-infused solution, you will typically consider some desired business
value and a given source of data. For example, the business objective states that "given
1000 tickets (problem reports), try to determine the nature of the problem automatically".
Don’t accept the given data as the only source of information. Instead, explore other
possible sources through the following heuristics.

• Exploiting implicit data

• Taking advantage of meta data associated with the data you were given.

• Consider implicit or explicit tracability and represent the data in such a way that
takes advantage of these relations.

• Structure contains information. Resist the temptation to lose structure in order to
  apply some ML algorithm. Maybe the data was exported and structure lost. Try in
  such cases to reverse engineer the structure.

We’ll elaborate on these heuristics here.
TBC:

• Explain the heuristics: "implicit", "meta data", "traceability" and "structure".

• Use all relevant data: Do NOT ignore structured data!

3.6 Is the training data representative of deployment data?

TBC:
Assumption underlying statistical machine learning: the training and test data distri-
butions represent the deployment distribution. In fact, many times the data is collected
in a totally different way than the data the system will encounter during deployment. For
example, if self-driving car is trained in different weather conditions or in different coun-
tries. Another example is that data collected is different due to problems in measurements
or different scales.
How to handle:
Missing data - The scale is different (camera is positioned higher), Use knowledge about
the data distribution to determine if the data meets reality
Domain knowledge:
If you know that percentage of fatal side effects is negligible and you get data that has 0.80 fatal side effects, then something is wrong with the data. Another example of domain knowledge. Breast cancer percentage in the population is around 0.5

Statistical relations on data:
Capture and monitor feature relations and behavior (min/max, correlation, . . . ) Hands-on:
Otherwise you need to design experiments so that you demonstrate that your model monotonically improves with new data as you know that the data will change over time and your data is not representative.

3.7 Get to a supervised learning problem

ML shines when supervised learning can be applied. It is more mature and has a stronger success record. It’s also an indirect indication that you are able to quantify a business objective that will be used in testing the system. Accurate labels are required for training and testing. The challenge is to identify appropriate labels for the data.

Two general heuristics apply:

- Choose a subset of the attributes in the data for the labels.
- Create an experiment that will generate desired labeled data.

TBC: To predict system performance, a labeled test set will be required.

3.8 Minimize manual labeling, instead utilize experiments, rules and boosting

TBC - minimize remove hyper parameters.
Chapter 4

Unit Test vs. System Test of ML Based Systems

Why do we need more than one model to build a system? Possibly, we can always feedback the entire data to the machine learning algorithm and produce the desired system? Let’s consider the following example.

Example 1. Consider a system that identifies the type of vehicle in an image. We desire a rough classification into land vehicles that requires a track and those that do not, boats, submarines and flying vehicles. The images have reliable meta data that clearly state if the vehicle is a land vehicle or not. We could create two possible systems. We could try and build a monolithic model by training a model using the images and their meta data. Another option is to create a model, $M_1$, that identifies boats, submarines and flying vehicles assuming that the input images are not land vehicles and another model, $M_2$, that identifies if the images are land vehicles that requires a track or not assuming that the vehicles are land vehicles. We will then compose the two models to get our system in the following way. We will check the meta data of the image to determine if the vehicle is a land vehicle or not. We will then apply $M_1$ if the image is not a land vehicle and $M_2$ if it is. Which of the options is better? As we assumed that the rule is reliable and it seems reasonable to assume that it is stable over time we can probably assume that the second system is much better. In addition, the learning task in the second case are easier as we have less labels to classify so we may achieve better generalization overall.

Exercise 4.0.1. What happens in the two cases if the vehicle is amphibious? Try different possible assumption on the meta data categorization and analyze how the two possible systems are likely to behave under your assumptions.

The example above demonstrates why a hybrid system composed of ML models and deterministic rules may be the ideal architectural choice. Another interesting aspect of system decomposition for ML based systems is that its design should be driven by the data available for learning. To see why, consider a system we would like to develop that assists in diagnosing a patient. There are many medical conditions and most of them are rare. Thus, we may have just a few examples for most of the medical conditions. As a result, it may prove impossible to train a ML model that successfully predicts that the medical condition is a rare medical condition. There are simply not enough examples for the ML to generalize and predict in the case of rare conditions! This is a special case of stratification or slices on the independent variables that do not have enough training examples. For example, we
may know that cities and neighborhoods are both independent variables, that will affect whether or not a child will graduate from school, but we do not have examples for some of the cities or neighborhoods for which we would like to apply the model. Thus, we probably cannot train a ML model to predicts on those combinations of neighborhoods and cities for which we do not have training examples. Instead, the general rules is that slices for which there is not enough training data should be handled in the old fashioned by developing deterministic rules that apply to them. Again, the result is a hybrid system.

**Exercise 4.0.2.** We know that for some \( a \in \mathbb{R} \) the system is of the form \( f(x) = Ax^2 \) for \( x > a \) and \( g(x) = Bx \) when \( x \leq a \). You are given a training set \( D = \{ (3, 9), (4, 16), (5, 25), (6, 36), (7, 49) \} \). Which of the following parameters \( a, A, B \) can be learned and why? Next, assume that \( a = 0, A = 1 \) and \( B = -1 \). Write a program that randomly generate data for the above case. Implement a learning algorithm that will learn \( a, A, B \) in this case. Generalize your data generating process so that it will randomly generate legal data for random choices of \( a, A, B \). Show that your algorithm learns for a random sample of data generated by your data generating program. Is your ML algorithm a composition of several ML algorithms or a monolithic solution? Why did you chose one solution over another and what were the trade offs that you took into account?

For regular systems components or units provide a well defined deterministic interface and they interact at the various levels of the system, create composed components and eventually obtain the desired system objective. Thus, testing for regular software consists of validating the expected deterministic behaviour of the system at each level of components composition.

For ML based systems, testing consists, in addition to traditional testing, of experiments on random performance variables that needs to be controlled at the different system levels. In addition, the random performance variables need not be the same at all levels of the system. We may thus be interested in the accuracy of intent classifiers of the chatbot solution at the unit level but the average number of service calls that are directed to a human agent at the system level (see chapter 8 for details). Thus, experiments need to be conducted at the unit and system levels to establish control over their their associated and typically different random performance variables. In general any component of the system that has at least one ML model embedded in it will require validation of control of some random performance variables through appropriate experiments.

As mentioned above, an interesting curiosity of the process of crafting ML based systems is that the optimal architecture is "driven by the data". Thus, experiments not only serve to test the system but also to design it. In addition, the line between testing and designing is blurred. We have seen how weakness in training data for slices of the data may drive the decomposition of the system. Such weaknesses are discovered through experiments. Thus, indeed, the results of the experiments and the data available drive the design of the system.

It is interesting to note that some view test first for regular software as a design paradigm. From that perspective the analogy between test first for regular software and experiment first for ML embedded systems is strengthen as both approaches are said to drive the design of the system.

**Exercise 4.0.3.** Consider a complete rooted binary tree of depth \( n \) (i.e., a path from the root to a leaf has \( n \) vertices). Each node in the tree represents a decision the software is making. In addition, assume the decision at node \( v \) of the tree has error probability \( p_v \). An adversary chooses a path, \( v_1, \ldots, v_n \) from the root \( v_1 \) to a leaf \( v_n \). A decision is then made
by the system by making a decision at each node of $v_i$ with error probability $p_{v_i}$. The system makes a correct decision only if all decisions along the path are correct.

1. What is the probability of making a correct decision if $v_1, \ldots, v_n$ is chosen by the adversary?

2. Which path should the adversary choose?

3. Implement an algorithm that finds the path the adversary should choose. What is its running time and is that the best running time possible?

A useful abstraction that applies to many ML based systems and will help us better understand the fundamental challenges of crafting ML based systems is a decision tree. The system is using the decision tree to make decisions. The nodes of the decision tree are decision point and can utilize either some deterministic rule or a ML model. If the ML model is used at a decision tree node to make a decision, the decision is correct in probability and its correctness probability may also dependent on the independent variables that govern the system. We refer to such a decision tree as the ML system hybrid decision tree. For a detail example of such a system see the chatbot example in 8. In that example the system uses intent classifiers to decide what the customer is interested in (paying a bill, withdrawing money from their account, etc), the system then proceed to follow a deterministic decision process that obtain the necessary data from the customer and complete the required service. Given a system with a hybrid decision tree, we can now elaborate on the challenges encountered in testing it as follows. We will refer below to nodes that use ML models to make a decision as non deterministic nodes and node that use rules to make the decisions as deterministic nodes.

1. Each non deterministic node performance dependent variables needs to be identified and statistically controlled through an appropriated experiment. Note that there could be more than one dependent variable to analyze per non deterministic node. For example, if the decision is whether or not to report some new drug side effect to the government, it may be more important that we report a true new side effect than that we do not report the new side effect when there is one. Thus, the two possible error types, namely reporting on a new side effect when it is not a new side effect or not reporting on a new side effect when it is a new side effect needs to be analyzed.¹

2. Is the hybrid decision tree the best way to design the system? Can we suggest a different hybrid decision tree that will better utilize the data and get a better overall performance or a more stable one?

3. Is the performance of the entire hybrid decision tree satisfactory? What are the performance variables that need to be analyzed for the entire system? These overall system performance variables need to be analyzed for each path in the hybrid decision tree that contain a non deterministic node. Some times we can deduce the analysis from the experiments on non deterministic nodes along a path (see proceeding exercises), but most likely we will need to conduct new experiments to test the entire path’s performance.

¹TBC - explain why you are not using standard terminology - false negative, false positive, precision and recall. Not everything is binary.
The following exercises are designed to clarify the concepts of unit test, system test, and system design using the hybrid decision tree for ML based systems.

Exercise 4.0.4. Developers developed a classification model as part of a larger system and wanted to test it. In order to do that they have obtained a new labeled data set, T, that is representative of the data that will be encountered when the model is deployed as part of the system and that was not used to develop the model. They calculated the accuracy of the model, i.e., the percentage of correct answers the model gave on T, and the number was 95% which seems to be a good number so they concluded that the model is validated.

1. The probability that the model is less than 93% accurate is required to be less than 0.05. Can we conclude that the model met this requirement?

2. Is there anything wrong with what the developers have done? Discuss your answer in light of statistical stability and system business requirements.

3. The classification problem is a binary calcification problem with two possible labels, -1 and 1. T has 1000 data points 500 of label 1 and 500 of label -1. On label 1 there are 10 mistakes and on label -1 there are 40 mistakes made by the model. What is the probability of mistake given that the label is -1 or given that the label is 1?

4. Every time the model makes a mistake on label 1 the company losses 100$ and when a mistake is done on label -1 the company losses 50$. What is the expected loss from a 1000 data points encountered by the system?

5. The data in production drifted and now we expect 900 out of a 1000 records to be of label -1. The model conditional probability of making a mistake on each of the labels (-1 and 1) remains the same. What is the expected loss of the company on 1000 data point encountered by the system now?

Exercise 4.0.5. To follow the experiment first approach, we use the following steps:

1. Identify a requirement and quantify it resulting in a dependent variable we want to analyze through an appropriate experiment.

2. Use domain knowledge to identify the independent variables that impact the above dependent variable.

3. Design an experiment that will predict the relation between the dependent and independent variables. The dependent variable will be estimated using the result of applying the ML based system or any of its components on the system inputs. Which part of the system is applied dependents on the level in which the test is conducted. In the hybrid decision tree model the test may apply to a non deterministic node in the tree or to the entire tree.

Consider the following questions.

1. Is there a difference in the statistical techniques that are applied to a non deterministic node in the decision tree or to a path in the hybrid decision tree?

2. Does it make sense to apply statistical tests to other parts of the hybrid decision tree (other than a path or a node)?
3. Consider your answer to the previous question. How would you define unit test and system test in light of your answer?

Exercise 4.0.6. Isaac Asimov defines his three laws of robotic in his 1942 short story "Runaround". The laws read

1. First Law. A robot may not injure a human being or, through inaction, allow a human being to come to harm.

2. Second Law. A robot must obey the orders given it by human beings except where such orders would conflict with the First Law.

3. Third Law. A robot must protect its own existence as long as such protection does not conflict with the First or Second Law.

Define a non deterministic decision tree that implements the above laws and is as "doable" as possible with the current state of the art of ML.
Chapter 5

ML Testing

AI infused systems are becoming embedded in our everyday life. This chapter outlines how to engineer AI infused systems reliably and confidently. It is challenging to build AI infused system that we can trust. Cutting to the heart of the matter: AI infused systems contains ML components. Such components are non deterministic and may sometimes make the wrong decisions. To handle that we introduce the scientific method and experimental design and explain how they are utilized to control the errors introduced by an AI infused system and thus make it trustable.

This chapter is organized as follows. We first introduce the problem of controlling AI infused system quality through an ideal and simple example and then deep dive into the scientific method, design of experiments and how they are used to develop, analyze and validate high quality AI infused systems.

5.1 Business grade ML solutions

As stated above we are going to discuss the creation of business-grade ML solutions. The objective is to create an ML solution decision makers can use to guide their decisions with confidence or even let the ML solution make decisions without a human in the loop. This is not new. For years statistics has been used to guide decisions and make them with confidence. For example, a production line is only profitable if up to 5% of its produced items are defective. We sample the production line every 20 minutes and determine the percentage of defective items in the sample. Apply a statistical test or a confidence interval that was previously developed we determine if production should be stopped and the production line re-tuned as there are too many defects making the current production not profitable. The decision is made at a certain confidence level as there are probabilities associated with the two types of errors that we can make; The first is that the production line is profitable when it is not and the second is that the production line is not profitable when it is.

We make the following crucial observation. ML solutions are a complicated version of the above production line example. They are heavily dependent on data and are random by nature. In other words, if a fresh training data sample is chosen the resulting ML model and its performance will change. Thus, repeating the learning process on two different samples of training data will probably produce two slightly different ML models. Also by definition sometimes ML models are correct and sometimes they are not correct! It’s the nature of the beast.

In order to achieve business-grade ML solutions we need to statistically control the solution error. The following is meant by statistical control. The solution performance,
say accuracy, is a random variable. We would like to be able to claim the following type of claim: with probability of error of no more than 5%, the accuracy of the solution lies between 84% to 87%. We call this interval a control interval as this interval is used to "control" the ML performance and determine if it is within the expected bounds.

In other words, we want to be able to say what the expected performance of the system will be and quantitatively determine the probability we will make a mistake. If we are able to do that we will also be able to determine if a ML solution is performing correctly in the field as we should rarely, if ever, see a performance that is outside the control interval.

Our approach as mentioned before is non parametric as for modern ML infused systems it is hard to determine a distribution family and fit a distribution to the data. Another motivation to the use of non parametric approaches is the availability of modern computers. Utilizing the computation power of modern computers we will be able to rely on approaches such as bootstrapping and Monte Carlo to develop our ML infused system’s control.

We will start by studying how to estimate any random variable distribution in a non parametric way. This will serve as the foundations for our first ideal control interval example.

5.2 Random variables empirical distribution

We are given a probability space $(E, \Omega, P)$, $\Omega \subseteq 2^E$ and a random variable $X : E \rightarrow R$. We define the distribution function $F : R \rightarrow [0, 1]$ by $F(x) = P(\{\omega \in E | X(\omega) \leq x\}) = P(X \leq x)$.

Example 1. Consider a fair dice. In that case, $E = \{1, 2, 3, 4, 5, 6\}$ which are the possible results of a throw of the dice. As $E$ is finite, all possible subsets of $E$ are possible events in the probability space. Thus, $\Omega = 2^E$. Set $X(i) = i, i = 1, \ldots 6$. We next have $F(3) = P(\{\omega \in E | X(\omega) \leq 3\}) = P(\{1, 2, 3\}) = \frac{3}{6} = \frac{1}{2}$.

Exercise 5.2.1. Calculate $F(i)$ for $i \in \{-1, 0, 1, 2, 5, 6, 10, 10.1\}$.

We are given a sample, $S = \{x_1, \ldots, x_n\}$ of the random variable, chosen randomly and independently from $E$. Next, we define the empirical distribution function, $F_n(x) = \frac{\sum_{i \in S} I(x_i \leq x)}{n}$ where $I(condition) = 1$ if the condition is true and 0 otherwise.

Example 2. Consider the fair dice again. Define the random variable to be $X(i) = 1$ if and only if $i$ is even and zero otherwise. Assume we got the following sample $S = \{0, 0, 1, 1, 0, 1, 0\}$. Then $F(0) = P(\{1, 3, 5\}) = \frac{1}{2}$ but $F_n(0) = \frac{\sum_{i \in S} I(x_i = 0)}{n} = \frac{4}{3}$.

Exercise 5.2.2. Write a simulation that obtains a large $S$ from a fair dice distribution. What is $F_n(0)$ converging to? Same question for $F_n(1) - F_n(0)$?

Example solution: Here

Recall that the Bernoulli distribution, $Br(p)$, is obtained by a trail that has success probability $p$. Success is denoted by 1 and failure by 0. For each point, $x_i$, in the sample $S$, $P(x_i \leq x) = F(x) = P(I(x_i \leq x) = 1)$. Thus, the random variable $I(x_i \leq x)$ is distributed Bernoulli with probability $F(x)$. Or $I(x_i \leq x) \sim Br(F(x))$. We thus have $E(I(x_i \leq x) = F(x)$ and $V(I(x_i \leq x)) = F(x)(1 - F(x))$.

Let’s pause here to better appreciate what have just happened. We are taking a non parametric approach. One of the fundamental patterns of non parametric statistics has just been realized above. The argument above applies for any distribution $F()$. Regardless, we have made an observation that connected the statistics of interest, in this case, $I(x_i \leq
x), with some known distribution, $Br(F(x))$, thus returning to the well known grounds of parametric statistics!

**Exercise 5.2.3.** Using the fact that $I(x_i \leq x)$ is distributed Bernoulli prove that $E(I(x_i \leq x)) = F(x)$ and $V(I(x_i \leq x)) = F(x)(1 - F(x))$. As a consequence what is the average and variance of $F_e$?

As a consequence $E(F_e(x)) = E\left(\frac{\sum_{i \in S} I(x_i \leq x)}{n}\right) = \frac{\sum_{i \in S} E(I(x_i \leq x))}{n} = \frac{nF(x)}{n} = F(x)$. $F_e(x)$ is thus an unbiased estimator of $F(x)$. In addition, $V(F_e(x)) = V\left(\frac{\sum_{i \in S} I(x_i \leq x)}{n}\right) = \frac{\sum_{i \in S} V(I(x_i \leq x))}{n^2} = \frac{nF(x)(1 - F(x))}{n^2} = F(x)(1 - F(x))$. The important point to note here is that as $n$ grows the variance of $F_e(x)$ vanishes making $F_e(x)$ an excellent estimate of $F(x)$.

Let’s take a deep dive into the behaviour of the empirical distribution.

**Definition 5.2.1.** We are given a sequence of random variables $X_1, X_2, \ldots$ with a corresponding distribution functions $F_1(), F_2(), \ldots$. In addition, we are given a random variable $X$ with distribution function $F()$. We say that $X_1, X_2, \ldots$ converges in distribution to $X$ at $x \in R$ if $F_n(x) \rightarrow F(x)$. If that is the case for each $x \in R$ for which $F()$ is continuous we say that $X_1, X_2, \ldots$ converges to $X$ in distribution.

**Exercise 5.2.4.** Consider the series of functions $f_n(x) = \frac{1}{n}(1 - \frac{1}{n})^2 x + (1 - \frac{1}{n})$, $n \in N$. Show that for each $n \in N$, the function $g_n(x) = f_n(x)$ if $\frac{1}{n} \leq x \leq 0$ and 0 otherwise is a density function. Also show that for each $x \in R$, the series $f_n(x)$ converges as $n$ goes to infinity to $f(x) = \frac{1}{2}x + 1$. Show that $g(x) = f(x)$ if $-2 \leq x \leq 0$ and 0 otherwise is also a density function. Is it also true that the random variables defined by $g_n(x) = \frac{1}{n}(1 - \frac{1}{n})^2 x + (1 - \frac{1}{n})$ converges in distribution to $g(x) = \frac{1}{2}x + 1$? If this is the case what needs to be proven?

Click here for a simulation.

### 5.3 Control interval example with unlimited sampling with replacement

We provide an example of obtaining a control interval for a ML model. We assume unlimited access to labeled data that represents data at deployment time. That is an ideal assumption. Much of our discussion in latter sections will focus on how to remove that assumption using bootstrapping and Monte Carlo techniques but the non parametric statistical approach will remain the same. As previously mentioned, We will be applying mostly non parametric statistics throughout this chapter as we typically do not know the type of probability distribution. This is another complication that is typical to modern ML work. An exception to this rule is when we are dealing with averages and large samples. The central limit theorem will then guaranty that the distribution of the average converges to the normal distribution and we’ll be able to use that to utilize parametric techniques.

We assume a model $f()$ was developed that given an image $x$ determines if $x$ is a dog or a cat. As we are given access to unlimited set of labeled data of cats and dogs that represents the data we will encounter when the model is deployed, we sample from the data and get a fresh set of labeled cats and dogs $(x_i, y_i), i = 1, \ldots, n$. $x_i$ are the images and $y_i$ is the label $y_i \in \{cat, dog\}$. We then calculated the sampled accuracy $a = \frac{\sum_{i=1}^{n} I(f(x_i) = y_i)}{n}$ where $I(c)$ is the indicator function that is equal to 1 if the condition, $c$, is true and zero otherwise.
We make the following observation. If we repeat the above procedure, and obtain a fresh random sample, we will get different results for the accuracy. Thus, accuracy is a statistic that estimates the real accuracy of \( f() \). In order to determine the actual accuracy with high confidence we need to develop a control interval. We proceed as follows. We repeat the above procedure \( k \) times and obtain \( k \) accuracy scores \( a_1, \ldots, a_k \). We order them in descending order, \( wlog, a_1 \geq a_2 \geq \ldots \geq a_k \). We take away 2.5% of the first numbers in the list and 2.5% at the end. The remaining numbers define the control interval. The accuracy will lie in this interval in probability 95%.

**Example 1.** We make the connection to the empirical distribution studied in the previous section explicit through an example. Assume \( k = 1000 \) and \( a_i = i \). Thus, 2.5% of the top will be the 25 numbers 1000, \ldots, 976 and the bottom 2.5% will be the the 25 numbers 1, \ldots, 25. According to the definition of the empirical distribution, \( P_e(a \leq 25) = \frac{25}{1000} = 2.5\% \), and \( P_e(a \leq 975) = \frac{975}{1000} = 97.5\% \). Thus, \( P_e(a > 975) = 1 - \frac{975}{1000} = 2.5\% \). It turns out that \( P_e(25 < a \leq 975) = 95\% \). As discussed in the previous section, when \( k \) grows that will be a better and better approximation of the unknown \( P() \) distribution.

**Exercise 5.3.1.** Repeat the example with \( k = 100 \) and \( a_i = i \). Be careful to handle the boundaries correctly.

**Example 2.** Click here for an example of a non parametric confidence interval. As the data is sampled from the normal standard distribution, and we take 2.2% of the largest and smallest points we expect the 96% confidence interval to be approximately \([-2, 2]\) when the sample size increases.

### 5.4 Bootstrapping

Bootstrapping is a way to overcome budget limitations. Ideally we would like to obtain a set of fresh samples as previously explained and obtain a confidence interval for the accuracy or other performance measure of the ML model using non parametric statistics. As discussed this is then used to anticipate and control the performance of the system in the field. Additional usage includes to compare models and determine if indeed one of them is better than the other or if the difference in their performance is a result of noise. We thus see that the techniques we are discussing here impact influence the end to end process of development of a ML solution. We deep dive into that the coming sections.

In practice we can not obtain unlimited number of fresh lab led data samples representing the field data. In fact, if we are lucky, we have one sample that represents the field data and is labeled. As long as this sample is not used for training the model we can use it to estimate the field behaviour of the model, but how do we overcome our budget limitation, namely, having only one sample? We follow the bootstrapping procedure to obtain new data samples. We call such data samples bootstrapped data samples. Technically, we repeatably sample with replacement from the one sample that we have to get our \( k \) samples and then proceed as before. To understand bootstrapping consider a data sample of blue and red balls. The probability of getting a blue ball is \( \frac{1}{3} \) but we don’t know that. If the data sample is big enough we will have roughly \( \frac{1}{3} \) of the balls being blue. This is the big "if" of bootstrapping - we require that the data sample distribution represents the real distribution. Now if we sample balls randomly from the data set we will get a new data set that will also have the \( \frac{1}{3} \) blue balls proportions. It is "as if" we have sampled a fresh sample where as
we actually sampled from our existing sample. This is the core idea behind bootstrapping. We can do that as many times as we like to get a set of "fresh" samples and then apply the non parametric procedure described in the beginning of the chapter for the dogs and cats classification example to obtain a confidence interval on the accuracy. We treat the bootstrapped samples as fresh samples hence the name "bootstrapping".

**Example 1.** Click here to see an example of a bootstrapping and non bootstrapping confidence interval for the balls. The expected range should be around $\frac{1}{2}$. Note that the sample size should be big enough in order for the bootstrap confidence interval to work.

**Example 2.** Click here to an example of trained models performance analyzed non-parametric confidence interval.

### 5.5 Using the central limit theorem instead

Given our idealized assumptions of independent random sampling with replacement the central limit theorem could have been applied as well in order to obtain a confidence intervals. In any case, it is a good idea to apply, if possible, more than one method to validate the confidence interval being developed.

Recall that the normal variable is close under linear transformations. Specifically if $X$ is normally distributed $N(\mu, \sigma)$ then $Y = aX + b$ is distributed with normal distribution $N(aX + b, |a|\sigma)$.

**Exercise 5.5.1.** Prove that if $X$ is normally distributed $N(\mu, \sigma)$ then $Y = aX + b$ is distributed with normal distribution $N(aX + b, |a|\sigma)$. Is that correct for $a = 0$?

The central limit theorem states that if $X_1, \ldots, X_n$ are sampled independently from an identical unknown distribution $F()$ that has a finite average $\mu$ and a finite standard deviation $\sigma^2$ then setting $S_n = \frac{\sum_{i=1}^{n} X_i}{n}$ we have that $\sqrt{n}(\frac{S_n-\mu}{\sigma})$ approaches the standard normal distribution, $N(0, 1)$, for sufficiently large $n$.

Setting $a = \frac{\sigma}{\sqrt{n}}$ and $b = \mu$ we get that $\frac{\sigma}{\sqrt{n}}(\sqrt{n}(S_n-\mu)) + \mu$ is distributed $N((\frac{\sigma}{\sqrt{n}})0 + \mu, (\frac{\sigma}{\sqrt{n}})1) = N(\mu, \sigma^2)$. In other words, $S_n$ is distributed $N(\mu, \frac{\sigma^2}{n})$. Thus, in order to develop a confidence interval we need to estimate the average and standard error of $S_n$ assuming it is normally distributed.

TBC - explain the difference between the two possible estimates to the standard deviation as $n$ is large it does not matter. Give a Python example.

**Example 1.** Click here for an example of how a large sample that is distributed normally can be used to estimate its average and standard deviation and thus obtain a confidence interval.
Chapter 6

Drift Detection and ML Solution Retraining

As previously mentioned, ML systems typically consist of input data and a target that is to be modeled or predicted on the basis of the input by an ML model. To the degree it is able, the ML model captures the relationship between the input and output target learned from training data. The model will then be deployed (used to generate predictions) on another set of input data. An underlying assumption of the exercise of building a model is that the input and target data in deployment will be similar to that in learning; if not, the model’s predictions may not be trustworthy, and its performance (e.g., accuracy) will be unstable and different than on the training data. What we call ‘drift’ will be changes in the underlying data, whether or not they cause the model performance to change.

This chapter is organized as follows. We will first introduce basic notions of the types of drift and their effects on the model. Then, we will discuss ways of detecting that drift has occurred, as well as some techniques to overcome these challenges. Lastly, we will mention some statistical issues that arise in drift detection. Since drift detection is a very wide topic, this is not exhaustive but will rather cover some basic concepts.

6.1 Types of drift

In general, let us denote the input data as $X$ and target as $Y$. $X$ can denote input data of any kind, such as embeddings of natural language and or image instances, or structured tabular data; $y$ can denote a class or numeric-valued feature, in which case the ML model is a classifier or regressor. Letting $p(\cdot)$ denote an arbitrary probability distribution, let $p(y \mid X)$ denote the true, unobserved, probabilistic relationship\(^1\) between the value of the predictor features $X$ and the target $y$; we aim to model $p$ by, say, some classifier model. If a given dataset $D$ consists of $X$ and $y$, the joint distribution of data observations in it can be denoted $p(y, X)$. This distribution can be decomposed\(^2\) as $p(y, X) = p(y \mid X) \times p(X)$, since the observations are assumed randomly sampled from an underlying population distribution $p(X)$.

Mathematically, drift between two observed datasets $D$ and $D'$, can be expressed as saying that $p(y, X) \neq p'(y, X)$, that is, their respective joint distributions differ. If we

\(^1\)The notation ‘$a \mid b$’ denotes $a$ conditioned on, or determined by $b$.

\(^2\)This follows from the laws of decomposing joint probability distributions into products of conditional distributions.
further decompose both as above, if there is drift, then either \( p(y \mid X) \neq p'(y \mid X) \), or \( p(X) \neq p'(X) \), or both. Figure 6.1 illustrates these for the case where \( X \) consists of two numeric features, displayed as a scatterplot of points; for each point \( x \in X \), its binary target class \( y \) is indicated by point being either hollow or filled. The curved line represents the decision boundary between the class distributions \( y \) represents an abstraction of \( p(y \mid X) \) in the case where the classes are separable.

In Figure 6.1, the left image shows the baseline \( p(y, X) \), with the other two showing different drifted \( p'(y, X) \). For illustration, imagine that the two features plotted are AGE (horizontal, say from age 16 to 65 years) and CREDIT RATING (vertical, where higher values indicate better credit), each point corresponds to an applicant for a student loan; the class \( y \) is the bank’s decision, indicated by the color of the point, with black being ‘reject’ and green being ‘approve’. Here we see that at younger ages, any credit rating will get you a loan (green), while as age increases, only the applicants with better credit will be approved, with the approval threshold increasing.

In the center image is what is typically called ‘concept drift’, where the relationship \( p(y \mid X) \), illustrated by the placement of the class decision boundary, has changed. In this case, it means that, say, a young applicant with a lower credit rating (lower left corner) would now be rejected when he previously would be accepted, since this point would now fall ‘under’ the decision boundary. In this image, \( p(X) \) has changed, since the points are located in different places, but \( p(X) \) could have also remained constant. The right image shows an example of ‘virtual drift’, where only the sampling distribution \( p(X) \) (point placement) has changed to \( p'(X) \). The decision boundary, however, remains the same as in the left image, meaning that a given input \( x \in X \) would still have the same class, since \( p(y \mid X) \) is constant. Drift has occurred in that \( p'(y, X) \neq p(y, X) \), but only through changes in \( p(X) \).

The intuition of distribution drift in Figure 6.1 can be extended to any input \( X \), whether higher-dimensional or non-numeric inputs like images, sound recordings, etc., however in these cases the distribution \( p \) may be difficult to characterize mathematically. Also, \( y \) can be a numeric target, like income in dollars, rather than a class, or consist of multiple target values per observation (multi-output).

We note that there is disagreement among practitioners as to how to precisely define terms for various types of drift. [15] represents one attempt to formulate coherent definitions. The joint \( p(y, X) \) can be alternatively decomposed as \( p(y) \times p(X \mid y) \), changing
the order of conditioning from that above. In [4], for instance, \( X \) represents a classifier’s measured confidence on an input image instance of class \( y \), and only \( X \) and \( y \) are observed, not the intermediate images, and drift in \( p(y, X) \) is detected. Here, the drift is induced by changing \( p(y) \) (introducing a previously unseen class) rather than \( p(X \mid y) \) (characteristics of handwriting of each digit).

### 6.2 Measuring distribution differences

In Section 6.1, we introduced drift as indicating \( p(y, X) \neq p'(y, X) \) when \( p(\cdot) \) and \( p'(\cdot) \) are determined on two different datasets (or samples) \( D \) and \( D' \). To determine if there is drift, we want to measure degree of difference or distance between the two sample distributions. Depending on the objective, a drift analysis may be conducted on one or more of the following:

- \( p(y) \) vs \( p'(y) \) (class label distribution)
- \( p(X) \) vs \( p'(X) \) or \( p(X \mid y) \) vs \( p'(X \mid y) \), for each \( y \) (overall or class-conditional data distribution)

Furthermore, we note that each dataset \( D \) is actually treated as a random sample draw from some theoretical unobserved ‘population’ dataset \( D \) (see [13], page 20) with associated distribution \( P(\cdot) \) (as contrasted with \( p \) or \( p' \)). For instance, in the example mentioned in Figure 6.1, \( D \) and \( D' \) may represent samples (say, of sizes 1,000 each) of loan applicants in the USA in the months of January and July, 2021, respectively. The respective populations \( D \) and \( D' \), with distributions \( P \) and \( P' \) respectively, are all such applicants in the USA in these two months; the samples were obtained because, perhaps, data on all such applicants (population) is not easily attainable. The sample distributions are considered estimates (notated *) of the respective population distribution; thus, we can say \( p = \hat{P} \) and \( p' = \hat{P}' \), meaning, for instance “\( p \) is an estimate of \( P \)”. Due to random sampling, if two sample distributions \( p \) and \( p' \) are drawn from the same population distribution \( P \), we would not expect that \( p = p' \) exactly. Instead, if we try to decide if drift were occurred, we want to avoid considering small differences that may be due to random sampling as ‘drift’. Rather, we typically try to make inferences such as the following: given \( p = \hat{P} \) and \( p' = \hat{P}' \), how likely is it that \( P \neq P' \)? That is, the question often tries to infer whether the two observed samples \( p \) and \( p' \) are different enough (more than by random chance) to indicate that the unobserved \( P \) and \( P' \) themselves are different. If they are, this is considered ‘drift’. This is the nature of statistical hypothesis testing (see [13], page 375).

Such statistical drift tests (typically called ‘two-sample tests’ since they compare two random samples for equality, rather than, say, evaluating one sample to a fixed baseline value or distribution) can be conducted if the distribution can be characterized mathematically. However, sometimes this cannot be done, and thus a measure of distance between the two samples \( D \) and \( D' \) can be measured. [1] (Q4) reviews some examples. Here, we will just cite these measures without detailed elaboration.

**Exercise 6.2.1.** Assume that \( X = \{ x \in \mathbb{R}^3 \mid x_1 \geq 0, x_1 + x_2 + x_3 = 1 \} \) and that \( y = \{-1, 1\} \). Assume that the model \( m \) is accurate iff \( x_2 \leq \frac{1}{2} \). The model was trained with \( p \) being uniformly distributed on \( X \). What is the accuracy of the model on \( p \)? Next, the distribution on \( X \) is shifted to be uniformly distributed on \( \{ x \in X \mid x_2 \geq \frac{1}{2} \} \cup \{ x \in X \mid x_3 \geq \frac{1}{2} \} \). What is
the accuracy of the model on the new distribution? What type of drift occurred in this case? Suggest a change to the problem conditions so that the other type of drift will occur.

6.2.1 Two-sample distribution difference measures on X

For univariate samples (X consists of a single feature), many tests exist. We also list the test name as it can be found in Python packages such as scipy ([18]). Given two samples $D$ and $D'$, sometimes one is interested to know if they have, say, the same mean or variance, rather than whether the whole distributions $P = P'$. In these cases, the two-sample Student T-test (scipy.stats.ttest_ind) is often used to detect differences in the mean; Bartlett’s test (scipy.stats.bartlett) or Levene’s test (scipy.stats.levene, if the samples don’t appear normally-distributed) can detect differences in variance. The Kruskal-Wallis (KW, scipy.stats.kruskal) tests for equality of medians. If the data X are binary, the means are proportions restricted to $[0, 1]$; in these cases, Yates’ difference-in-proportions test ([19]) can be used.

If one wants to determine the likelihood of $P = P'$, and not just equality of summary statistics, often nonparametric tests are used; these tests make minimal or no assumptions about the shape of the distributions. Some common ones for continuous data are Kolmogorov-Smirnov (KS, scipy.stats.ks_2samp), Cramér-von Mises (CvM, scipy.stats.cramervonmises_2samp), or Anderson-Darling (AD, scipy.stats.anderson_ksamp); the AD test can test simultaneous equality of $k > 2$ samples, not just two. If testing equality of the distributions of orderings of values (rather than the distributions over the values themselves), the Mann-Whitney test (MW, scipy.stats.mannwhitneyu) is often used. Say, for instance, each of $D$ and $D'$ is associated with a separate team, and the values are the times in minutes that each racer on the team finishes a race; assume that the winners are determined only by the relative order they finish and not by the absolute times. In this case, the MW test indicates if the racers in the two teams are approximately evenly-matched in terms of the order.

The tests mentioned so far, like many others, rely on p-values, or significance levels (see [13], page 375) to make a decision. The null hypothesis ($H_0$) in each case is specified as equality of either the distributions $P$ and $P'$ or the statistic of interest; a low p-value, below a pre-specified $\alpha \in (0, 1)$, indicates that drift is likely because the distributions differ significantly. Because the statistical significance measured by p-values is known to have methodological issues, measures of effect size ([13], page 692), which more closely capture the magnitude of practical difference between the two samples’ summary statistics. Some commonly-used measures are Cohen’s $d$ and $h$ measures ([6]) for testing two-sample differences in means and binary proportions. These measures are compared to specified thresholds rather than an $\alpha$ value, to make a significance decision.

The local kernel-density-difference test from [7] (implemented in R as the ks package, [8]) identifies regions where the two densities $p$ and $p'$ differ significantly, as opposed to simply if they differ. An illustration on univariate data, with Python implementation, is shown in [1] (Q9).

For multivariate samples, the distributions are often harder to characterize easily, except in certain parametric cases like multivariate-normal, without making distributional assumptions. Wasserstein (also known as “Earth-mover’s”) distance measures the distance between two distributions using transport theory, representing each observation as, say, a grain of sand that must be moved’ from $p$ to $p'$. The more ‘distance’ each ‘grain’ must be moved to transform $p$ into $p'$, the greater the distance between them. These metrics
are implemented in Python as `scipy.stats.wasserstein_distance` (univariate case) and `ot.emd` (multivariate). Another nonparametric kernel-based distance is Maximum Mean Discrepancy (MMD, [10]); this is illustrated in [1] (Q4).

6.2.2 Two-sample distribution difference measures on \( y \)

In addition to the tests mentioned in Section 6.2.1 on numeric-valued input data \( X \), we can also test whether the distribution of observed labels \( y \) differ. Again, this determination is often made by assuming unobserved population distributions \( P \) and \( P' \). Because the values \( y \) are nominal-valued (categorical), such as the state (e.g., Alabama, Alaska, . . . , Wyoming) of residence of the loan applicant, \( P \) typically takes the form of a multinomial distribution ([13], page 208). The multinomial distribution \( M \) is denoted \( M(\pi, N) \), where \( N \in \{1, 2, \ldots \} \) is a positive integer representing the sample size (number of observations), and \( \pi = [\pi_1 \ldots \pi_k] \) is a \( k \)-length vector where \( 0 \leq \pi_i \leq 1 \), \( \forall i = 1, \ldots, k \), and \( \sum_{i=1}^{k} \pi_i = 1 \). Without lack of generality, let the \( k \) potential label values be \( \ell = \{\ell_1, \ldots, \ell_k\} \). \( M(\pi, N) \) models \( N \) label values, drawn independently, where each draw takes the \( i \)th label \( \ell_i \) with probability \( \pi_i \). Since all that is modeled is the total count of each label, and not the order, a vector \( x = [x_1, \ldots, x_k] \) can be modeled as a draw from \( M(\pi, N) \), if each \( x_i \) is a non-negative integer and \( \sum_{i=1}^{k} x_i = N \). That is, \( x_i \) is the observed occurrence, out of \( N \), of label \( \ell_i \). Therefore, given two observed label vectors \( y \) and \( y' \), where the corresponding counts vectors are \( x \) and \( x' \) (assuming both have the same size \( N \)), we can determine if they appear to come from the same multinomial distribution \( P \).

Probably the most-used test for equality of categorical counts is the one-way chi-square goodness-of-fit (`scipy.stats.chisquare`), not to be confused with the chi-square test for independence performed on a contingency table. This test requires the sums of \( x \) and \( x' \) to equal (\( N \) is the same). However, it is a one-way test, since one of \( x \) or \( x' \) must be set as the ‘expected’ and the other as the ‘observed’ values, which affects the calculation; in contrast, in the two-way tests, there is no ‘baseline’, and the order of specification of samples does not matter. This test returns a p-value used in the drift decision. An alternative is to use the effect size metric Cohen’s \( w \) ([6]), where the inputs are the values of \( x \) and \( x' \) divided by their sums, rather than the counts themselves.

6.3 Drift in characterizations of data

In Section 6.2, we presented a series of two-sample statistical tests, distance, and effect-size measures to detect distributional drift between two datasets \( D \) and \( D' \). There, we assumed we could, or desired to, model the dataset or label distributions directly. However, sometimes it is desired to model intermediate ‘aspects’ of the data, or a model’s performance on it, and detect drift on these aspects instead. We present several examples here.

6.3.1 Drift in data slices

Letting \( D \) and \( D' \) be tabular structured datasets of numeric or categorical features. [2] introduces the notion of a data ‘slice’ rule as a conjunction of subsets of a group of feature; a subset on a feature is an interval with a minimum and maximum value if the feature is numeric, or a set of potential values if it’s nominal. For instance, an example of a slice \( S \) is \{\( \$30,000 \leq \text{INCOME} \leq \$60,000 \) \& \{\text{STATE} \in \{\text{New York, Ohio, Michigan}\} \& \{\text{SEX} \in \{\text{Male}\}\}\}, which is defined on the three features INCOME, STATE, and SEX. An observation
falls in a slice if its feature values satisfy all conditions in the slice; for instance, any males with an income in the range $30,000–$60,000 and living in either New York, Ohio, or Michigan. The size, or support of a slice on a dataset of $N$ total observations is the number of observations falling in the slice; the fractional support is the support divided by $N$. Given a classifier model that returns predictions on $D$, [2] present an algorithm to find a set of such slices where specifically the classification error rate of the model is higher than the average over $D$; such slices are called ‘error-based slices’.

Given two similar datasets $D$ and $D'$ and the classifier’s predictions on each, [5] presents a method for detecting drift between $D$ and $D'$. The drift is not detected directly on the datasets’ feature distributions $p(X, y)$ and $p'(X, y)$, but rather by extracting a set of error-based slice rules on $D$, and detecting differences between this set and the rules when mapped to $D'$. Note that the $K$ slices can overlap in that an observation can fall into more than one of them. If $K$ slice rules are extracted, $\hat{\pi}_{1,i}$ and $\hat{\pi}_{2,i}$ be the observed fractional support of the $i$th slice out of $K$ on datasets $D$ and $D'$, respectively. If there is no drift between $D$ and $D'$, we expect $\hat{\pi}_{1,i} \approx \hat{\pi}_{2,i}$; the same is true of all $K$ slices. A difference-in-proportions test ([(19), mentioned above in Section 6.2.1]) can be used to test this; since $K$ hypotheses, one for each slice, are conducted, we have $K$ p-values $p_1, \ldots, p_K$.

Ultimately, we want a single decision of drift over all the slice p-values, and not just to see if each slice individually has drifted (changed in size). This is done by using an adjustment for multiple comparisons (see [13] page 424), specifically Holm’s method ([(11)]), which produces a single p-value with a statistical guarantee on the familywise error rate (FWER) of the decision (i.e., across the ‘family’ of multiple hypotheses).

In this example, [5] used an ‘indirect’ drift test based on the set of slices, which has several advantages. First, it allows repurposing an existing technology for slice-extraction ([(2)]) for drift detection; this method can be used in other settings where ‘useful’ observation subsets can be defined. Second, since the purpose of the slices was to locate concentrations of model errors by the feature values, the technique allows detection of drift specifically in these areas, which are particularly useful because they indicate likely changes in model accuracy, assuming stability of the slice rules, and not just drift in the feature distributions. Thirdly, and most importantly, distilling the dataset into the simpler aspect of slice rules, which are now modeled by the univariate measure of proportion, simplifies the analysis from the multivariate case of actually modeling all the feature distributions.

### 6.3.2 Drift in density-based slices

[3] present a way to partition a dataset $D$ into a set of slices, which are defined in the same way as in [2]. However, here the $K$ slices extracted differ from [2] in two ways. First, they form a partition, in that together they contain all observations in $D$ and that each observation belongs to exactly one of them (as opposed to [2], where there may be overlaps and observations that do not fall in any of the slices). Second, these slices are constructed to contain observations with similar ‘spatial’ density within the feature space, rather than classification error; furthermore, some slices may defined feature subsets that are empty, containing no observations.

As discussed in Section 6.3.1, this method distills the feature space of $D$, which may be high-dimensional, into the lower-dimensional abstraction of useful slice rules. Furthermore, as in [3], though not discussed there, these slices can be used for drift detection in a similar way by testing differences in univariate measures, such as their fractional support or volume.

For instance, say the $K$ density-based slices on $D$ can be categorized as either ‘not very
sparse’ (type A), ‘very sparse’ (type B), or ‘empty’ (type C); the sparsity threshold can be decided based on, say, the average core distance, or slice volume divided by fractional support (see [3] for details). In \( D \), observations must fall only into either slices of type A or B, since those of type C are by definition empty. Now, let each observation in another dataset \( D' \) be mapped to one of the \( K \) slices. Then, each observation in \( D' \) can fall into one of either types A, B, or C. In addition, there is a new type, D, meaning that an observation contains at least one feature whose value is outside of the ranges observed in \( D \); for instance, a higher income than the highest observed in \( D \), or a country of origin not observed in \( D \). Similarly to in [5], if there is no drift in feature distributions between \( D \) and \( D' \), we may expect each type A, B, C, or D to have similar fractional support on the two datasets. Significant drift in these proportions—after an adjustment for multiple hypotheses—may indicate drift. Furthermore, this drift is easily explainable, in that we can point to which type (A, B, C, or D) changed the most, and identify some of the anomalous observations.

### 6.3.3 Drift in feature polynomial relations

Given a tabular dataset \( D \) of only numeric features, [17] present a method to extract strong polynomial relations from it. Say that the input data \( X \) contains \( m \) features, denoted \( X_1, \ldots, X_m \). A polynomial relation is a polynomial ‘equation’ between, say, \( X_1 \) and some \( k \) (e.g., 2) of the features, allowing feature interactions up to a limited degree \( \ell \) (say, 2). For example, \( X_1 \approx 2 + 3X_2 - 5X_2X_3 + 1.5X_2^2 \); let us denote this relation \( L_1 \). The relation between \( X_1 \) and the expression involving \( X_2 \) and \( X_3 \) is found using linear regression; hence the \( \approx \) symbol means that this is not a strict equality, but that there is some error, which is measured by the error term of the linear regression equation. Strong relations are polynomials where the regression coefficient of determination \( R^2 \) is high, indicating a strong linear correlation between the true value (e.g., \( X_1 \)) and the ‘prediction’ of the polynomial on the other features \( X_2 \) and \( X_3 \).

Given a polynomial \( L_1 \) determined on \( D \), we can see how good its fit is on the same features in another dataset \( D' \); in the absence of drift, we expect the fit to be about the same. The degree of change in fit is quantified by the Bayes Factor of \( L_1 \) on \( D \) vs \( D' \). In experiments with simulated drift insertion in [17], it is shown that for relations that had high initial \( R^2 \) (strong), the Bayes Factor was more responsive to drift insertion than weaker relations; that is, the strong relations were better indirect sensors of feature drift. Since many relations can be extracted from \( D \), a correction should be done to adjust for the multiple comparisons performed.

As in the previous examples discussed above, drift analysis based on the relations, rather than \( X \) itself, can be simpler. [17] suggest constraining the relations by \( k = \ell = 2 \), to prevent over-fitting and so they are relatively human-interpretable. The logic of drift detection here is that a strong relation is likely a fixed aspect of the data that should be stable; for instance, we may expect a person’s SALARY to have a fixed polynomial relationship to their years of EXPERIENCE and EDUCATION, and if this changes, it may indicate an underlying feature drift. In particular, if an ML model is to be be deployed on \( D' \), its performance may differ significantly from on \( D \) if there is drift, if the model exploits existing feature correlations for its predictions. Even if the intermediate relations themselves are not of interest, they can still be used as ‘detectors’ of drift.
6.4 Sequential drift detection

So far, the statistical tests and examples of indirect drift detection (Section 6.3) dealt with a single decision on $D$ vs $D'$. In many cases, however, we may observe an ordered sequence $D_1, D_2, \ldots$, often ordered in time, and want to determine if any differ from the initial $D$. 
Chapter 7

Optimal Integration of the ML Solution in the Business Decision Process

As previously discussed ML embedded systems are non deterministic. They make mistakes by design. What we hope to achieve instead of a bug free system is a system for which the error on the choices we want to utilize in the business decision process is statistically controlled. Such control enables the appropriate allocation of human resources for the correction of errors made by the ML embedded system and the insurance that overall we obtain a stable process that increases the profit of the organization. In addition, the way the ML embedded system is used may need to be updated over time as the factors impacting the performance of the ML embedded system may change. The last issue, drift identification, was dealt with in chapter 6 while the question of statistical control was studied in chapter 5.

The ML embedded system is integrated in a business process and should help increase value obtained from the process by the organization. For example, there are many consideration involved in reaching a decision of whether or not to give a loan to a bank’s customer. One of the consideration is if the loan payments to the bank will occur on time. Assume that we have developed a ML embedded system that predicts if the loan will be paid on time by a given customer. We want to integrate the prediction of the system in the overall decision process followed by the bank. The embedding should be made in such a way that the bank will maximize the profit from giving loans to customers. Giving loans that will be paid on time and not giving loans that will not be paid on time can help maximize the overall bank profit but this is not the only consideration. Other considerations may apply and influence the final bank decision. For example, if the bank can get the payments for the loans by other means such as accessing the customers assets. Let’s spell out two fundamentally different ways in which we can integrate the ML system in the business process.

1. If we can trust the recommendation of the ML system we can just act according to the recommendation. For example, a software problem is reported. The software is composed of components. Each component has an owner that can solve problems of the component that she owns. If we can trust the ML system to route the software problems correctly most of the time we can just route them automatically according to the ML recommendation. As long as the routing recommendation made by the ML system is mostly correct the value from the business process is clear as we no longer
require a team to route the software problems to the appropriate component.

2. The ML system recommendation is correct most of the time but cannot be "blindly" trusted. In our problem routing scenario a person is required to consider each ML recommendation. This can still be beneficial as given the recommendations, especially if the ML system provides the reasons for the recommendation, the time required to route each software problem is reduced.

3. A hybrid case. There are some conditions in which we have established, through an appropriate experiment, that we can trust the ML system "blindly" and some conditions for which we need a person to inspect the recommendation and make the final decision. A simple example of that is if we have established that for some software components we can route the problem report automatically according to the ML system recommendation and for some components we cannot and a person should make the final decision.

If the ML recommendation is not followed blindly (cases two and three above), a person sometimes should make the final decision taking into account the ML recommendation or potentially ignoring it all together. In this situation whether or not the person makes a correct decision depends on the incentive defined by the organization. Thus, as part of the optimal business definition process, if there are decision points in which a person needs to make a decision while taking into account a ML system recommendation that cannot be fully trusted, optimal incentives should be defined for that person. This calls for the application of mechanism design, see link. We will attempt to get a better understanding on how this can be achieved in practice in the next section.

7.1 Business process optimization and incentive design

We start with an example of optimization of the business process associated with the ticket routing ML embedded system. The ML embedded system uses several models and utilizes different parts of the problem report such as the report text and the report meta data. In addition, the system may utilize other sources of information such as the software installation configuration. Finally, the system may also use some deterministic rules based on certain error codes. For example, if out of memory error is reported route the problem to the memory management of the software. As discussed in chapter 4, the ML system is thus typically composed of a hybrid decision tree. We are emphasising this as one may think the assumptions we are making next only apply to a single model and they typically do not. Hence the consistent use of the terminology ML embedded systems throughout this work.

We assume that the software has four components, namely, \( c_1, c_2, c_3, c_4 \). Previous experiments have shown that the average conditional probability of correct routing decision given that the decision is one of the components \( c_1, c_2, c_3, c_4 \) is \( P(\text{correct} \mid c_1) = 0.6, P(\text{correct} \mid c_2) = 0.7, P(\text{correct} \mid c_3) = 0.8, P(\text{correct} \mid c_4) = 0.9 \) respectively. A human resource is available that can analyze the problem and correctly route it at the cost of 1 unit. We are also given that the observed probabilities of reporting a problem by the ML system from each of the components \( c_1, c_2, c_3, c_4 \) is \( \frac{1}{4} \). The average performance of the system if the human resource is not used is thus \( \sum_{i=1,2,3,4} \frac{1}{4} P(\text{correct} \mid c_i) = 0.75 \). We consider applying the human resource only in case that the system predicts \( c_1 \) which we refer to as the elimination of \( c_1 \) policy. On the average that will be a quarter of the time, so on the average we expect to pay 250 units of payments in a 1000 software problems. What is the
expected performance of the joint business process that utilizes the human resource in that way? It is expected to be completely correct for \( c_1 \) thus \( P(\text{correct}|c_1) = 1 \). We will have the average performance of \( \sum_{i=1,2,3,4} \frac{1}{4} P(\text{error}|c_i) = 0.85 \). We thus increased the average performance of the system from 0.75 to 0.85 at a cost of 250 units of cost in a 1000 software reported problems. This highlights the trade-off involved in applying the human resource. Consider the following exercise to better understand the concept.

**Exercise 7.1.1.** Assume the routing problem as explained above.

1. What will be the average performance if we only eliminate policy \( c_2 \)? Same question for policy \( c_3 \) and \( c_4 \)? What are the average costs in that case?

2. We randomly choose to apply the human resource in probability \( p \). What will be the average performance of the system and the average cost in this case?

3. You are given a budget of 100 cost units per a 1000 software problems how would you spend it? What will be the average performance then?

4. What is the standard error of an elimination policy \( c_i \) given that we know that the standard errors of each of the conditional probability \( P(\text{correct}|c_i) \) from previous experiments? How would you check the stability of an elimination policy?

5. What will be the impact of change in the probability of the ML system reporting a problem in a components. For example, what will be the impact of the ML system reporting a \( c_1 \) problem in probability 0.7 and \( c_2, c_3, c_4 \) in probability 0.1 each? Assume the conditional probabilities of the ML system being correct given the component prediction stays the same. Explain why such a phenomenon is possible?

6. What will be your recommendation if you do not have an estimate of the probability in which the ML system will choose one of the components? Explain.

We can thus consider a general category of policies, namely elimination of \( c_i \) given that the ML system recommended routing to \( c_i \) in probability \( p_i \). The expected accuracy in such a case will be \( \sum_{i=1,2,3,4} \frac{1}{4}(p_i + (1 - p_i)P(\text{correct}|c_i)) \). We denote this expected accuracy by \( P(\text{correct}|p_1,\ldots,p_4) \). We can think of our problem as the problem of maximizing \( P(\text{correct}|p_1,\ldots,p_4) \) under a given budget constrain. We are ensured that this optimization problem has a solution. See next exercise for details.

**Exercise 7.1.2.** Show that \( P(\text{correct}|p_1,\ldots,p_4) \) is continuous and that the set of possible utilization of the budget constrain, e.g., if the budget is 250 cost units per a 1000 software problems and is utilized so that \( \frac{1}{4}(p_1 + p_2 + p_3 + p_4)1000 = 250 \), is compact. Deduce that the optimization problem has a maximum. See appendix for details on why this is the case.

In a way the above approach to the problem is the simplest possible approach as either the ML embedded system is making the routing decision or the human resource does. Concerns are thus "separated". We can measure the performance of the ML embedded system when its decision is trusted and separately measure the performance of the human resource when she makes the decision on the routing. In other words, for each routing decision there is a single "owner", either the ML embedded system or the human resource. Next we consider a more hybrid scenario in which the two are brought together to make the final decision.
Assume that the human resource spends up to some time bound on the routing decision and that the accuracy is proportional to the time spent. For example, assume that the human resource spends up to 2 hours on the routing decision and that the accuracy of routing of a decision that was made after $t$ time is $\frac{t}{2}$. The cost now of applying the human resource is the overall time that the human resource spent on making routing decisions. We also assume that other assumptions on the routing problem and the ML embedded system remain the same. Assume that the overall time the user can allocate for 1000 software problems is $T$. The human resource can perfectly handle $n = \frac{T}{2}$ routing decisions (ignore the reminder). One approach could be to assume that we have $n$ cost units as before and solve the previous optimization problem.

**Exercise 7.1.3.** Assume the routing problem described above. Further assume that we would like to raise the average accuracy from 0.85 to 0.9. One way to achieve that would be to spend $0.9 \times 2$ time on each routing decision for which the ML embedded system recommended $c_1, c_2, c_3$. This will raise the the conditions probabilities $P(\text{correct}|c_i), i = 1, 2, 3$ to 0.9. How big should $T$ be to implement this approach?

We now consider the problem of incentive. We observe that there are two different type of decision makers. The first design the overall business process. For example, decides what type of elimination policy to choose in the problem routing example. The second decision are the decision made by a human resource that participate in the decision process. In our routing problem example the human resource making the routing decision. The first principle of incentive definition is to tie incentive to the the part of the organization business goal controlled by the decision maker. In our ticket routing example the decision maker that optimizes the entire business incentive should be tied to the entire business process performance. For example, in the ticket routing example the business process optimizer should be rewarded for a decrease in the overall time required to solve problems, a decrease in the overall expense required to solve the software problems, and so on. In contrast, the human resource used to route software problems only controls the correct and efficient routing of a given software problem. Thus, she needs to be rewarded in proportion to volume of correct routing and in reverse proportion to time it took her to make the decision. Note to provide such incentives the organization will need to measure the performance of the system. This should be thus part of the system requirement and experiment design from day one of the ML embedded system development!

**Exercise 7.1.4.** Consider the bank loaning example. Assume that two ML embedded system are developed. The first estimates if a loan will be return on time by a customer with accuracy 0.8. The other ML embedded system estimate if a customer will increase her business with the bank as a result of given a loan. There are budget con trained human resources that can make the two decisions. The bank is expanding so if the business with the customer is likely to increase and the customer is likely to pay the loan the bank policy is to given it. Define appropriate optimization process and incentives for the business process optimizer and human resource decision maker. Make additional assumption as needed similar to the one made in previous exercises of this chapter.
Chapter 8

A Detailed Chatbot Example

8.1 Chatbots as a ML embedded system

Chatbots are becoming a key channel for customer engagement. Chatbots are automated systems through which users can interact with the business through a natural language interface. For many customers, the chatbot provides their first interaction with the business and serves as the ‘face’ they meet—and their first impression. Automation that can create a positive and rich customer experience, and enable repeat business, must be able to ‘understand’ the customer as a human would and respond accordingly. However, many chatbots fail to provide a high-quality customer experience because they do not understand the customer’s intent, are not designed to cover enough situations, or even fail to respond appropriately to the user request. To provide the best possible customer experience, the chatbot has to be reliable, be consistent, interpret user intents correctly, and respond appropriately. The chatbot has to respond by comprehending the underlying intent behind the users’ utterances. This is something that can only be ensured through comprehensive training and testing that is geared specifically to the chatbot’s business performance, its conversational responses, and interactions.

Chatbot technology usually comprises two basic components, as shown in Figure 8.1:

1. A machine learning (ML) natural language processing (NLP) based intent classifier that can process what the user is saying, and

2. A conversation flow orchestrator that incorporates domain knowledge and is driven by the business actions and content extracted from past human-to-human dialogs and company documents. Typically the orchestrator is rule base and does not apply use ML.

This chatbot architecture may be represented as a non deterministic tree. The ML models that classify the user intents (item 1 above) typically occupy the upper levels of the non deterministic decision tree. The rule-based flow orchestrator (item 2 above) typically occupies the rest of the tree and is deterministic.

Exercise 8.1.1. An online shop sells home repair equipment for householders and professionals. A model, \( m_t \), was developed that identifies if a customer is a preferential or a householder. Another model, \( m_a \), determines if the customer would like assistance in the use of some equipment. Additional models, \( m_h, m_p \), were developed that give recommendations for additional purchase for householders and professionals respectively. Finally, a model \( m_c \) was developed that determines if the customer would like to complain about an equipment
that was purchased. There is a rule based system, \( r(m_t, m_n, m_w) \), that handles the customer requests. Design a non deterministic decision tree that utilizes the above ML models and the rule based system. Determine the expected accuracy of each path in the decision assuming the accuracy of the trained ML models are given.

8.2 Quality challenges

Testing a chatbot requires assessing not only the quality of the classifier but also the end-to-end conversation including the subsequent intermediary system actions (business functions) that complete the conversational interaction. This testing must be carried out in the pre-deployment stage, before the chatbot is deemed production worthy. Of course, the testing is also needed once the chatbot is in production, to check for functional consistency and monitor for continuous improvement. As with any ML solution, it will need periodic evaluation and testing to flag recalibration and the need for adjustments.

The big challenge of chatbot development lies in getting enough quality data to train the chatbot and test it thoroughly in the first place. This is more problematic if the chatbot has yet to interact with customers, meaning there is no history of interactions and conversations to use as a test bed. The trainer or the tester of the system must be able to provide enough sentences that can predict what the users will say at runtime. This is challenging. Usually very little data is available to test or even train the chatbot. There exist powerful data augmentation technologies that can help overcome this challenge.

Depending on the level of business logic one may want to develop, building a simple question-answering bot can be pretty straightforward. But, a more serious investment of
resources is needed to enable the bot to deal with more complicated user queries. When clients, and customers of clients, are exposed to an early or low-quality version of a chatbot, their perception and satisfaction will be affected by its quality.

The nature of human language makes it impossible for software tests to cover all possible situations. Although websites and smartphone apps use predefined interactions based on common user interface components like buttons, hyperlinks, or text-entry, the integrated chatbots have to cover both the directed or expected and the unexpected or free format conversational variations. This is where the importance of comprehensive testing comes in.

Testing should begin early in the solution life-cycle. This is fundamentally different from the complementary activities of analyzing the system once it is deployed for continuous improvement and retraining. The data that is available is much more limited in the testing phase, and does not include real user interactions. For example, actual contextual variables for input that needs to be identified during the flow are mostly provided when real conversations exist. The majority of data available in the testing phase is related to the machine learning task of classifying those first important user utterances into the correct category of intent. This is the training and/or test data for the intent classifier. To provide reasonable coverage, this data must be extensive and representative of real user interactions with the chatbot.

While conversation flow modeling also needs to be developed early on, it is based primarily on the input of the person developing the virtual assistant. Once the virtual assistant has been released to users, there exist actual conversation logs. These logs can then be analyzed to understand which conversations were abandoned and why. This data also provides an opportunity to analyze conversations that went wrong and improve the conversation flow and the intent classifier based on user interaction.

It is important to develop approaches to predict such un-handled conversation flows based on the data available during testing. The idea is to provide the system with examples of challenging utterances so the chatbot developer can improve its design and implementation even before the first release.

8.3 Control for chatbot success

TODO ¡¡Ateret lets do it together¡¡

Monitoring completion status during operation is needed in order to measure the actual chatbot system business value. This is different from monitoring the intent classifier accuracy. One can can view this as system level monitoring vs. unit testing.

8.4 Trend analysis

When a chatbot is released to users there is data of conversations and their completion status. Un-handled logs, or traces from those human-chatbot interactions that did not succeed, are of special interest.

In addition to improving the chatbot training data and potentially also design, un-handled logs may be an indication of actual changes, trends or drift. These changes may be due to changes in the environment or in the topics. There is a need to understand when changes are intermittent and should actually best be ignored, and when they indicate change of trend or drift and should be accounted for, for example by retraining the ML models.
Covid-19 questions provide an example. At the beginning of the pandemic most questions to Covid-19 related chatbots were around asking for information about the pandemic. Then as governments published restrictions, questions changed to be around the nature of the restrictions. When vaccines were developed, questions changed yet again to be around the vaccines and related recommendations and warnings.

The reader is referred to Chapter 6 for a comprehensive discussion of drift and its identification and ML models.
Appendix A

Solutions

Here are a list of solutions to selected exercises.
Following is the solution to 2.0.2.
Appendix B

Annotated References

Here we briefly discuss some references on the crafting of reliable ML embedded solutions. In [9] a general motivation for assurance of ML embedded systems is given.
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