Aging Prediction of Single Base Propellants through Machine Learning Methods Integrated with Genetic Algorithm

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Aging Prediction of Single Base Propellants through Machine Learning Methods Integrated with Genetic Algorithm

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Dedications

"To my father, who is no longer with me to witness me complete my work. May I have the same unwavering dedication to my field in science that you had in me."

Abstract

The prediction of aging and serviceability in single base propellants has become remarkably effortless owing to the rapid advancement of new analytical techniques, specifically High-performance liquid chromatography (HPLC). However, HPLC only provides momentary situations. To address this issue and to obtain real time aging prediction of SBPs this research explores the use of machine learning (ML) and genetic algorithms (GA). Aging refers to the deterioration of the propellant over time, which can affect its functionality and performance. The study uses predictive ML models to optimize, automate, and surveil single-base propellants in combination with GA to enhance their performance. Widely used machine learning models include support vector machines (SVM), ensemble trees (ET), Gaussian process regression (GPR), and regression trees (RT). Several criteria are used in this study to evaluate the models' accuracy and probability for prediction. The study is significant with 0.89 coefficient of determination for the optimum performing ML technique namely ET-GA to forecast the effects of aging on propellants, contributing to the advancement of testing and surveillance techniques for single-base propellants. An optimized ML model ET-GA shows maximum of 5% deviation with experimentation is used to create a Graphical User Interface (GUI) that simplifies the calculation of the remaining effective stabilizer percentage.

Keywords: Propellants, Energetic Material, Nitro Cellulose, Machine Learning, Genetic Algorithm.

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Nomenclature

Single Base Propellants	SBPs
Machine Learning	ML
Genetic Algorithm	GA
Remaining Effective Stabilizer	RES
Support Vector Machine	SVM
Gaussian Process Regression	GPR
Ensemble Tree	ET
Regression Tree	RT
Graphical User Interface	GUI
Nitrate Ester Plasticized Polyether	NEPE

Chapter 1:

Introduction

1.1 Background

When ignited or detonated, highly energetic nitrogen-based compounds known as propellants quickly release significant amounts of energy and gaseous byproducts. They are extensively used by the military and by the construction and mining industries [1]. Several aging reactions, including nitrate breakdown and post-curing reaction can degrade propellants with time. Scholars have used chromatography, spectrum analysis, mechanical analysis, thermal analysis and computer simulations to evaluate and predict the extended storage effectiveness of propellants. Propellant's lifespan is often estimated to be between 13 and 16 years [2].

The materials used as propellants in rockets, missiles, and other propulsion systems create thrust. Early in the 20th century, researchers began looking into different chemicals' capacities to generate regulated propulsion for use in the military and space applications. One of the first propellants used was black powder, which has its roots in ancient China. However, the present rocket business underwent a revolution when liquid and solid propellants were developed in the middle of the 20th century.

Fuel and oxidizer are combined to form a solid matrix to form solid propellants. Solid propellants first appeared in gunpowder, but Dr. Robert Goddard's research in the early 20th century led to their modern formulations[3]. Solid propellants are the best choice for both industrial and military applications since they are straightforward, portable, and simple to handle.

Although they offer many advantages, propellants also have significant disadvantages. Propellers may degrade over time for a number of reasons, such as environmental exposure and chemical instability. Their performance and safety may be significantly impacted by this decline. For instance, the propellants' combustion properties may alter over time, impacting the amount of thrust produced and trajectory control. The structural integrity of the rocket engine may also be in danger as a result of cracks or cavities developing inside the solid propellant grain as a result of degradation [4, 5].

Recently, engineers and researchers have concentrated on improving propellant compositions to extend their shelf life and improve stability. Research has been done to examine the mechanisms of deterioration and develop strategies to halt or slow the process. These efforts have led to the development of more dependable and long-lasting propellant formulae, ensuring the efficiency and security of modern propulsion systems.

Propellers must be maintained and stored properly to preserve their performance and avoid early deterioration. Proper storage procedures, regular inspections, and adherence to safety procedures are required to maintain propellant integrity throughout its useful life.

Propeller degradation-related safety problems can be a big problem. A rocket might malfunction, for instance, if a propellant deteriorates to the point where it delivers insufficient thrust. A propellant may potentially explode if it deteriorates to the point that it becomes unstable. These are the causes for propellants to require meticulous upkeep and routine inspection for signs of deterioration. Propellers should be stored in a cool, dry area away from air and moisture. Furthermore, it is vital to regularly check propellants for deterioration indicators such fractures and discolouration [5].

1.1.1 Single Base Propellants

The present work proposes a new method that combines genetic algorithms (GA) and machine learning (ML) to forecast the aging of single-base propellants (SBP). The majority of propellants are SBPs, which find utility in everything from rocket propulsion to missile propulsion systems. SBPs primarily consist of plasticized nitrocellulose (NC), which is used as both a fuel and an oxidizer, with a tiny mass percentage of additives such stabilizers and plasticizers [6-11].

SBPs have a number of benefits over other propellants because of their high energy densities. They are a popular option for many applications since they have strong storage stability and are relatively simple to handle. But its sensitivity to heat and shock, which can result in an early ignition or detonation, is one of their biggest drawbacks [12]. The instability and susceptibility to thermal stress of the CO-NO bond can be attributed to its low binding energy (155 kJ/mol) [13-15].

1.2 Aging in Propellants

Aging in SBPs is a natural process **(Figure 1)** that refers to the deterioration or changes that occur over time in the physical, chemical, or mechanical properties of a propellant, which can affect its performance or functionality. Several variables can affect the breakdown of a propellant, such as its initial composition, conditions during its production, and external conditions during storage. These factors may affect how quickly and how decomposition proceeds**.** Propellant decomposition products, such as NO and NO2, accelerate further propellant decomposition. This can eventually lead to declining physical and ballistic properties [16-19]. Aging directly affects the storage life (shelf life) and service life. [18].

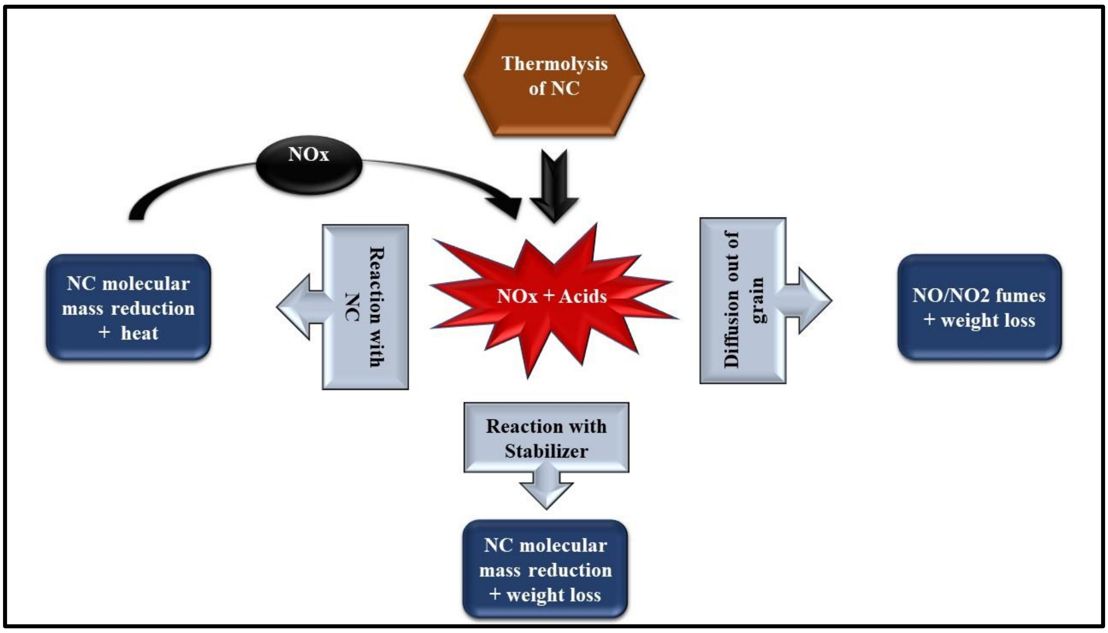

Figure 1: Schematic showing chemical aging of propellant.

1.2.1 Diphenylamine

To scavenge nitrogen oxides and slow nitrogen ester decomposition, stabilizers are added to propellants [20]. By preventing nitrocellulose (NC) from degrading on its own, diphenylamine (DPA) is frequently employed as a stabilizer in single-base propellants (SBPs) to increase their chemical stability [21]. Nitrated analogs of DPA are formed because of decomposition (N-NO-DPA, 2-NDPA, 4-NDPA) and they also act as stabilizers [10, 22, 23] **(Figure 2)**. The stabilizer composition ranges between 0.5% and 2% of the total mass% **(Table 1)**. For propellants to remain stable, regular monitoring of stabilizer content or surveillance testing is essential. A minimum of 0.2% DPA is typically used as the lower limit [13, 24]. According to Allied Ordnance Publication – 48 (AOP-48), if the effective stabilizer percentage of a propellant is lower than 0.2%, it must be considered unserviceable. If the DPA content exceeds 3-4%, it may also result in incompatibility [25].

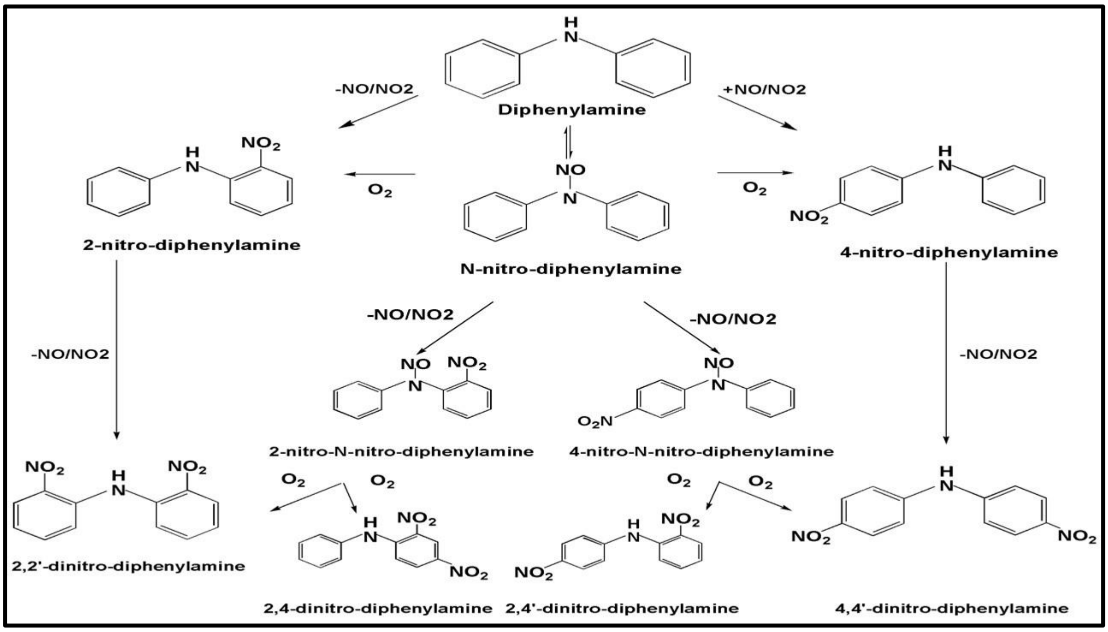

Figure 2: Sequential degradation of DPA.

Table 1: Composition of SBPs

S. No	Chemical Composition	Mass%	Function
1.	Nitro Cellulose (N – Content)	90 – 95%	Main Energy
2.	Diphenyl Amine (DPA)	1 – 2 %	Stabilizer
3.	Dibutyl Phthalate	2 – 5%	Plasticizer
4.	Graphite	0.2%	Burn Rate Enhancer
5.	Moisture	0.6 %	Mechanical Strength

Since certain nitrate-derivatives of DPA are used as stabilizers, it is essential to figure out the “remaining effective stabilizer” (RES) which is a combination of the original stabilizers and N-nitroso-diphenylamine content [24, 26]. Researchers have established that the reduction of stabilizers is not only dependent on temperature but is also affected by many variables including temperature, relative humidity, moisture content, and initial composition [19, 27-31].

1.3 Surveillance Testing

The Hansen-Metz test, the red fumes test and methyl violet test are just a few of the techniques that have been devised to assess the chemical stability of NC-based propellants. These monitoring and stability tests have been devised to ensure the reliability of the propellants [15, 18, 32-34]. Surveillance testing is an essential aspect of the quality control and safety of SBPs and is typically conducted during various stages of the propellant production, storage, and use. The surveillance of gun propellants involves either examining their thermal behavior or measuring their RES content [17, 35].

In the present study, the deterioration mechanism was monitored through employment of high-performance liquid chromatography (HPLC) by scrutinizing the RES% [36]. It may be noted that serviceability and aging of propellants is directly dependent on RES %. HPLC tests carried out to analyze the serviceability of NC-based propellants are in accordance with the NATO Standardization Agreement (STANAG) 4620 and Allied Ordnance Publication (AOP) 48 [26, 37]. It may be noted that HPLC gives a momentary situation. HPLC data can be helpful in gauging the stability of propellants, but it cannot determine how long they will remain usable when stored [38, 39].

Surveillance testing has been used since ages however, in the era when the world is moving towards smart automation and Industry 4.0 [40], it offers certain disadvantages such as time and cost, human error during sampling, limited scope, false sense of security, and inability to comply with regulations [41].

Chapter 2:

Literature Review

2.1 Literature Review

The amount of literature relating to propellants and the application of machine learning techniques within this domain is quite sparse, according to a preliminary search conducted on the Google Scholar platform. However, there has recently been a steady increase in publications in this sector, which can be linked to a growing interest in the investigation of novel and improved energetic materials that are suitable for a variety of use cases.

Some of the most dynamic domains of inquiry in energetic materials and propellants encompass [42-44]:

- new energetic material synthesis and characterization
- modeling and simulation of the behavior
- the burning and ignition of combustible materials
- Safe handling of materials
- uses for energetic materials in explosives, pyrotechnics, and propulsion

Research in these areas enables the development of the most advanced energetic materials and propellants, and contribute towards the development of new and improved materials with improved performance, safety, and environmental impact [45, 46].

Artificial intelligence (AI) has progressed in different areas over time. AI has been used in military operations, space exploration, medical care, and other tasks. AI is designed to imitate human behavior to reduce costs and save time [47]. Energetic materials has undergone major modifications as a result of the big data era's advent [48-50]. Since the invention of black powder the development of energetic materials has mostly relied on conventional trial-and-error approaches [50, 51]. Over the past few decades computational chemistry have matured enough to complement and aid experimental studies [52]. AI is much more than a rule-based program; it uses sophisticated ML models that are backed by experimental data and scientific computation. This makes AI an effective, highly developed and reliable approach [53, 54].

This study examined how ML can be used to predict the aging of SBPs, based on their RES. For this research, predictive ML models are used to gain insights from the data thus increasing the efficiency and monitoring of SBPs. These models provide a practical solution that can be used for optimization, automation, and surveillance.

Various ML techniques were used to forecast SBP aging. As illustrated in Figure 3, a machine learning model was employed that incorporates several input variables, including initial composition, temperature, relative humidity, and moisture content. These variables include nitrocellulose (NC), moisture (M), hygroscopicity (H), dinitro toluene (DNT), graphite (G), methyl violet test at **134.5°C** (MV), DPA, zone (Z), Temperature (T), humidity and propellant age.

For research, different ML models were coupled with GA, an optimization method for designing a predictive ML model. By integrating ML with GA, prediction of the effects of aging on propellants was carried out more accurately. This can be beneficial for further research on double- and triple-base propellants. Multiple machine learning models, including support vector machine (SVM), ensemble tree (ET), gaussian process regression (GPR), and regression tree (RT), were used to train the data. The machine learning model's parameters were adjusted using a genetic algorithm (GA) to facilitate further optimization. The formulation of a Graphical User Interface (GUI) using MATLAB improved the precision of aging predictions. A comparison between the machine learning model's projected values and the investigational results was done to verify the effectiveness of the model.

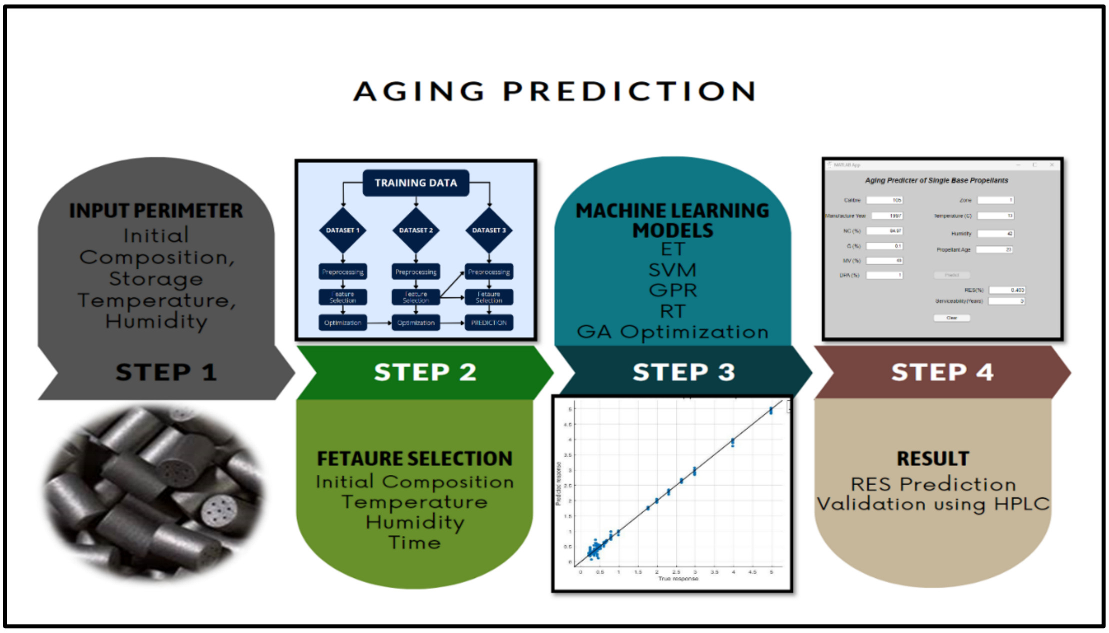

Figure 3: Steps involved in aging prediction.

The current surveillance testing procedures for SBPs are mostly dependent on the relationship between temperature and relative humidity using an empirical formula, rarely paying attention to the history of stabilizer depletion under different environmental and storage conditions [55-57]. For this research, DPA content histories of propellant samples at various moments in their life were obtained; the initial DPA contents were also known. Samples were collected from different temperature zones to perform a comparative analysis.

2.2 Objectives

The following are the primary aims of the current investigation:

a. A feature selection approach for the ageing of single base propellants was conducted through employment of a genetic algorithm (GA).
b. Partial dependence analysis of the input parameters on the propellants ageing.
c. Prediction of ageing using optimized ML methods integrated with GA.
d. Influence of various parameters on propellants ageing.
e. Efforts are being made to create a graphical user interface (GUI) that will forecast the deterioration of propellants in real time.
f. Validation of the proposed model with the experimental results using HPLC.

2.3 Research Justification and Relevance to National Needs

There is a noticeable dearth of published research on the utilization of artificial intelligence methodologies for the purpose of predicting propellant aging, and as a result, designing an interface that can effectively forecast aging in real-time. It is crucial that we maximize artificial intelligence (AI) and ML to develop a wireless or non-invasive mechanism capable of accurately forecasting propellant aging in the context of changing environmental factors like temperature, humidity, chemical composition, and other pertinent variables. This research will prove to be economically viable and in accordance with the United Nations Sustainable Development Goal no 9 and a step towards modernization.

Potential energy policy and economical constraints are important motivators for ML based aging prediction of propellants, particularly in developing nations such as Pakistan. The aging of solid propellants can seriously affect their mechanical and chemical properties [58]. Therefore, it is crucial to make accurate predictions regarding the aging of propellants to ensure their safety and optimal performance. The implementation of machine learning techniques can significantly enhance the reliability of lifetime predictions for energetic materials. With the help of this novel methodology, composites' structural characteristics and combustion behaviors, which have a significant impact on their overall performance, may be accurately forecasted [59]. Knowing ahead of time the anticipated lifespan of different energy materials is beneficial from an economic point, as well as for performance and safety. Energy-dense materials tend to age rapidly when kept at elevated temperatures, which could result in thermal instability, leading to failure or unintended ignition. Machine learning approaches can be used to anticipate the aging of propellants in order to get a deeper understanding of the physical elements of combustion processes and to pinpoint the variables that affect the pace of burning. This may ensure the safe and efficient use of propellants, which may be advantageous.

2.4 Thesis Outline

The thesis aims to explore the challenges and opportunities in integrating machine learning methods and optimization techniques with surveillance testing methods like HPLC analysis. Chapter 1 of thesis will focus on the background and existing surveillance methods. Chater 2 will begin with a comprehensive literature review, analyzing previous research on aging of propellants. Chapter 3 will provide an overview and will delve into the analysis of the existing machine learning and optimization techniques identifying key bottlenecks and limitations for aging of SBPs. Novel solutions developed will be critically evaluated for their efficacy in facilitating the more accurate aging prediction in Chapter 4 and 5.

Chapter 3:

Machine Learning Models and Optimization Algorithm

3.1 Machine Learning Models

Several ML methods, such as GPR, ET, SVM, and RT, were used to develop the best model for predicting SBP aging to meet our research goals. It was based on an estimate of how long the propellants had been subjected to different storing conditions based on the storage temperature, relative humidity, initial composition, and time since production. The optimum hyperparameters for the GPR and ensemble techniques were selected using Bayesian optimization. Training and evaluation were carried out using MATLAB software.

3.1.1 Support Vector Machine

For both classification and regression analysis, the Support Vector Machine (SVM) supervised learning model is used. It's a robust algorithm for machine learning that's adept at performing tasks such as outlier detection, as well as linear or nonlinear regression and classification [59]. The underlying concept of how SVM works is to determine the hyperplane that most effectively separates the data into different categories. By identifying the hyperplane that optimizes the distance between the two classes, this is achieved in a linear SVM. The margin is the separation between the nearest data points from each group, referred to as support vectors, and the hyperplane [60].

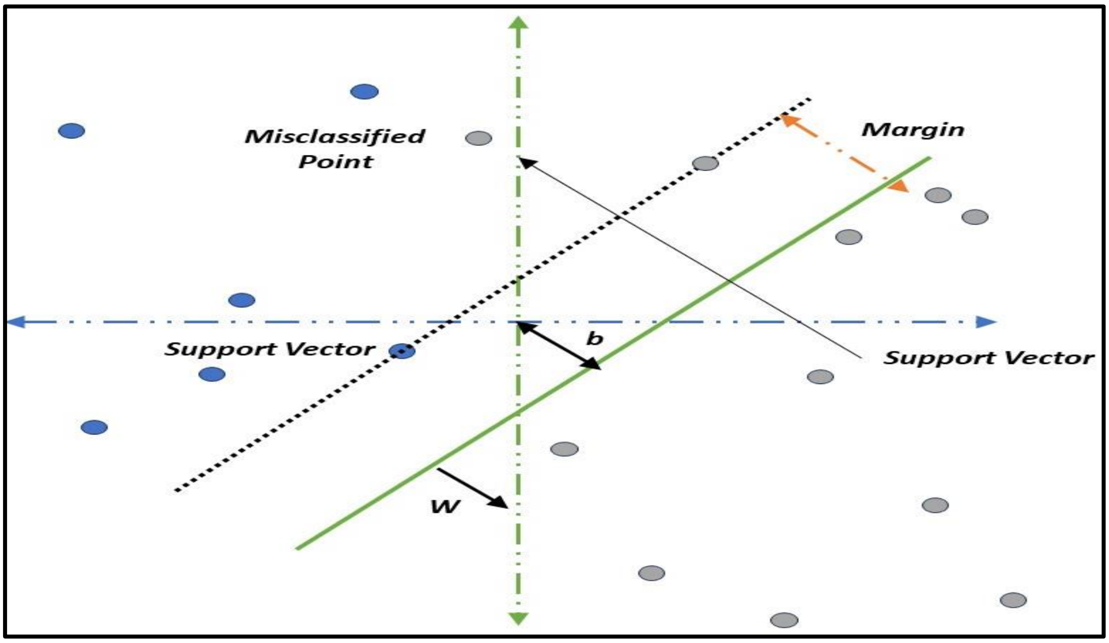

Figure 4: A graphical representation of SVM Hyperplane

SVMs have a number of advantages, including being very effective in high-dimensional environments, being able to handle circumstances in which the number of dimensions exceeds the number of samples, and using very little memory because they only need a small number of training points (referred to as support vectors) while making decisions. SVMs may integrate a range of alternate kernel functions into their decision-making process, which further increases their adaptability [61].

3.1.2 Ensemble Tree

An Ensemble Tree (ET) is a machine learning technique that utilizes multiple decision trees to enhance the precision and reliability of forecasts [62]. Ensemble methods are exceptional supervised learning algorithms that deliver remarkably precise solutions by training numerous models [63].

The concept at the core of the ET functioning is to merge the forecasts of different base estimators made using a particular learning method to enhance generalizability and resilience compared to a lone estimator. In general, ensemble methods belong to one of two categories: Averaging methods aim to create multiple estimators independently and then average their individual forecasts. The combined estimator, owing to its reduced variance, typically outperforms any individual base estimator. Bagging techniques and forests of randomly selected trees are two examples. In contrast, base estimators are constructed progressively in boosting approaches, and the bias of the composite estimator is attempted to be reduce [64].

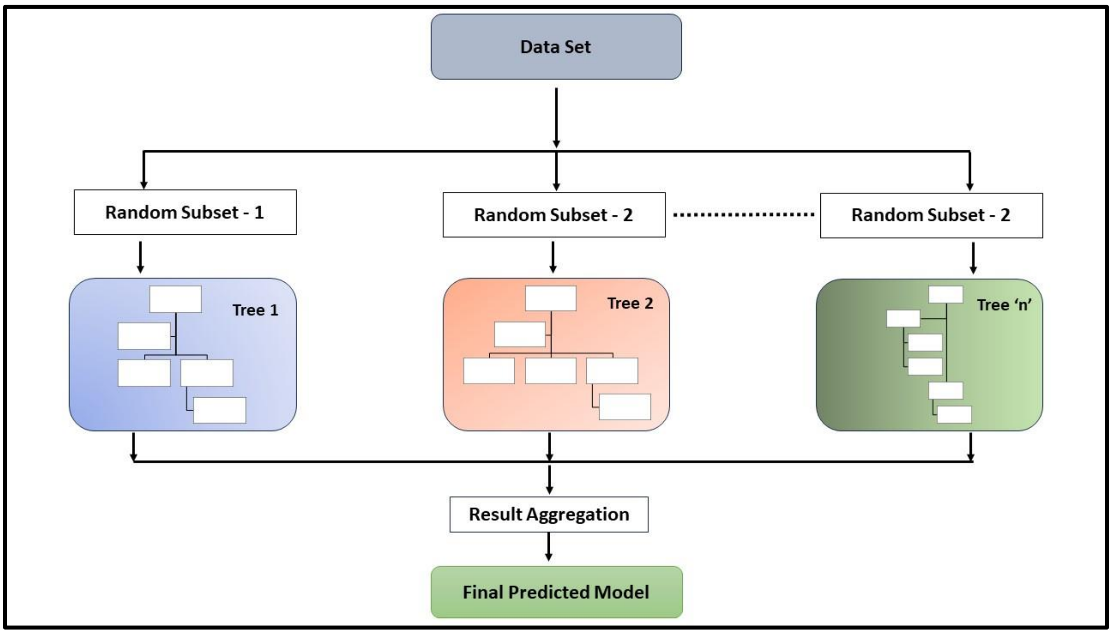

Figure 5: Bagging Training Procedure - ET

ET have many advantages, including their unmatched performance in high-dimensional spaces, their amazing capacity to handle scenarios in which the number of dimensions exceeds the number of samples, and their exceptional memory efficiency, which comes from their use of a subset of training points from the decision function (called support vectors). The fact that several kernel functions can be given for the decision function makes ET very flexible [64].

3.1.3 Gaussian Process Regression

The outstanding non-parametric Bayesian method known as Gaussian Process Regression (GPR) is widely employed in the field of machine learning. It is a straightforward approach for nonlinear function regression that requires little previous knowledge. In contrast to previous techniques, Gaussian Process modeling provides a mean forecast as well as a measure of the model's accuracy [65].

The fundamental principle underlying GPR is founded on the assumption that observations conform to a stochastic process that is normally distributed. Consequently, it can be inferred that subsequent observations do not modify the probability distribution of earlier ones in any way. Through this basic attribute, GPR facilitates the prediction of values that are not yet known [66].

3.1.4 Regression Tree

Regression trees (RT), a specific type of decision tree, are used to predict a continuous target variable. It can be used for applications in both classification and regression [67]. The fundamental idea that drives the functionality of a Regression Tree is to iteratively divide the data into increasingly smaller subsets, until they become sufficiently minuscule to be characterized by a straightforward model, typically a fixed value. The tree is formed by picking the most optimal split at each node, relying on a splitting criterion, such as reducing the total squared errors between the forecasted and factual values [68].

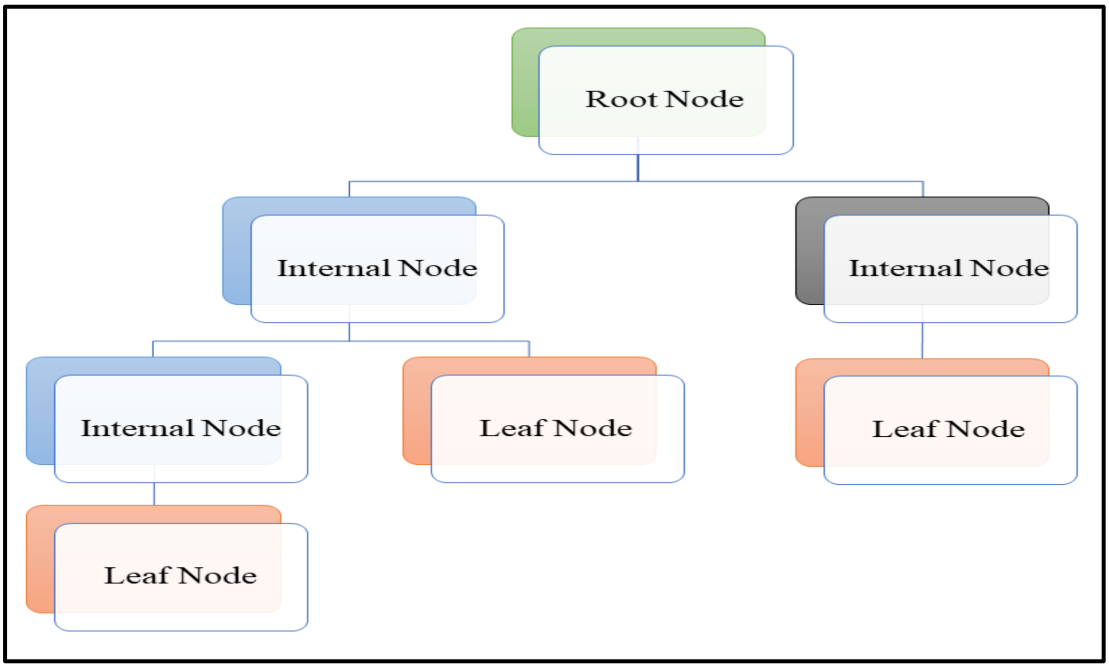

Figure 6: Regression Tree Analysis in Machine learning.

Some advantages of utilizing RT consist of their simplicity and ease of interpretation. They may be viewed and compared to actual trees since they have a root node at the top, branches, and terminal nodes (or leaves) at the bottom of the plot. Additionally, they require minimal data preparation and can handle both numerical and categorical data. Furthermore, they are capable of handling multi-output problems [67].

3.2 Optimization

3.2.1 Genetic Algorithm (GA)

The best feature selection and hyperparameter adjustment were carefully selected utilizing GA. To achieve the best results, we compared various optimization techniques. The GA is a method for search and optimization that mimics the process of natural selection seen in biological evolution. The GA operates in three steps: crossover, mutation, and selection. [69]. By testing and developing a set of candidate solutions iteratively, GA can be used to optimize an ML model. This approach, also known as a metaheuristic, is frequently used to come up with effective solutions for issues relating to search and optimization [70].

The general steps of GA for model optimization are as follows:

- Create a population of potential solutions, often at random.
- Determine the performance metric or goal function that best describes each solution in the population. The GA parameters at all these stages are with 100 generation. Scattered crossover technique is used with 80% probability and elite count of 4. Population type is bitstring with 50 size and uniform mutation is used with 10% probability**.**
- Create a new population by selecting the best candidates, generally using methods like crossover and mutation that were inspired by biological processes.
- Determine the population's level of fitness.
- Keep going through steps 3–4 until a good answer is discovered or a predetermined stopping criterion is satisfied.

Using GA, one may swiftly navigate through a sizable search field and find the best solutions to difficult optimization problems. The goal of the GA is to iteratively evaluate and improve potential solutions to identify the optimal one for a particular issue. The key advantages of the GA are its speedy discovery of nearly optimal solutions, robustness against noisy or imperfect data and capacity for handling enormous datasets [71].

In a GA, the fitness function is a crucial component that defines the optimization problem being solved. It determines how well each population's chromosomes represent a solution and guides the decision of which parents will have the next generation of children. The likelihood that a chromosome will pair with genetic material to produce offspring is determined by its fitness value [72].

Chapter 4:

Methodology

4.1 Methodology

The approach to research and framework used to answer the study questions and objectives are provided in full in the methodology portion of this thesis. This chapter outlines the systematic procedures and tools utilized for data collection, data analysis, and the interpretation of findings. The chosen methodology is grounded in established research principles and aligns with the nature of the study, ensuring the reliability, validity, and generalizability of the results. Additionally, potential limitations related to the research are discussed. By meticulously detailing the methodology, this chapter aims to provide a transparent and replicable foundation for the investigation, allowing readers to understand the methods utilized and the rationale behind their selection.

For this part of thesis data comprising initial composition of propellants their storage conditions, age and data available on surveillance test for serviceability of propellants was collected and preprocessed using different techniques available. Multiple ML learning models were integrated with GA to optimize prediction.

MATLAB R2021 was used for the above processes. Work methodology is shown in **figure 7**.

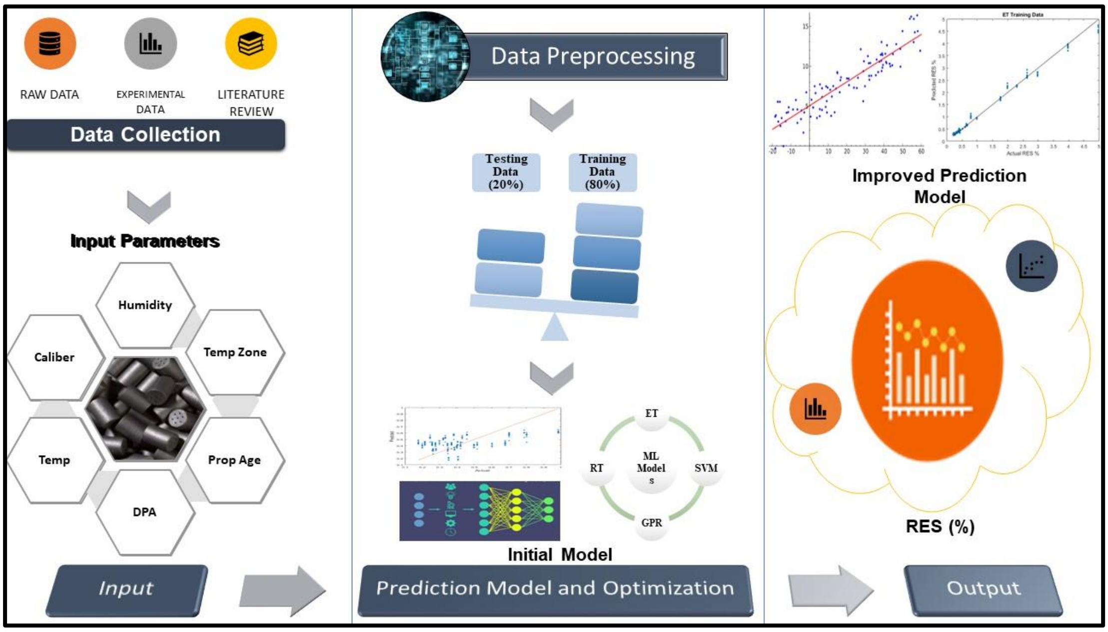

Figure 7: Research Methodology

4.2 Data Collection

A detailed survey of the published literature has been carried out for this research, focusing on the degradation of stabilizer content in SBPs. HPLC results for the RES were also obtained from different organizations, keeping records of propellant aging in Pakistan as part of the surveillance testing of SBPs. The major criteria for the collection of data revolve around the storage temperature of the propellant, relative humidity, and initial composition along with environmental conditions.

Data was collected in following steps: -

- By gathering surveillance testing data from various organizations, a total of **372** data points were obtained.
- Information was supplemented by data in the literature.
- Initial composition, storage temperature, relative humidity, year of manufacture and age of propellants (years since manufactured) were used as input parameter.
- MATLAB was used for preprocessing data.
- Cleaning and filtering of data was performed by removing or imputing missing values, removing outliers, and smoothing the data where necessary.

- Various filling methods like mean/median/mode imputation, forward/backward fill, linear interpolation, and k-nearest neighbor imputation were used.
- RES was the output parameter.

MATLAB provides several built-in functions to perform these preprocessing steps, including load, fill missing, isoutlier, smoothdata, selectFeatures, zscore, normalize, trainTestSplit, and encode Labels. The development of a GUI using the MATLAB toolbox facilitated the assessment of RES content for predicting the aging of SBP. This GUI simplifies entering the required information and allows for the visualization of the predicted RES values, making it user friendly for individuals.

Chapter 5:

Results And Discussion

The research's findings are reported and critically examined in the results and discussion chapter of this thesis in relation to the study's goals and the body of prior literature. This chapter goes into great detail about the methodology, experiments, and data analysis outcomes that were employed in the study. The results are carefully structured and supplemented with the pertinent tables, graphs, and visual aids to make them simpler to understand. The identification of significant patterns, trends, or relationships in the data that support the study's findings is also covered in this chapter. This chapter attempts to provide a critical examination of the research findings and their consequences, offering insightful commentary and opening the door for additional fieldwork.

5.1 Box Plot Representation of Input Values and Output RES

Quartiles, Q1, Q2, Q3, represent the minimum, medium and maximum values, which are used as the five-number summary in a box plot, also known as a box-and-whisker plot, to offer a visual representation of a dataset. This kind of plot efficiently depicts the distribution of data values and offers information on a dataset's symmetry, skewness, variance, and outliers. In a box plot, the first quartile through the third quartile is represented by the boxes, and the median is shown as a line inside the boxes. In addition, whiskers are discernible between each quartile and the minimum and maximum data values [73].

When examining the distribution of numerical data values between various groups, box plots are a valuable tool for presentation. They offer valuable insight into the symmetry, skew, variance, and outliers of a dataset, providing high-level information at a quick glance [74].

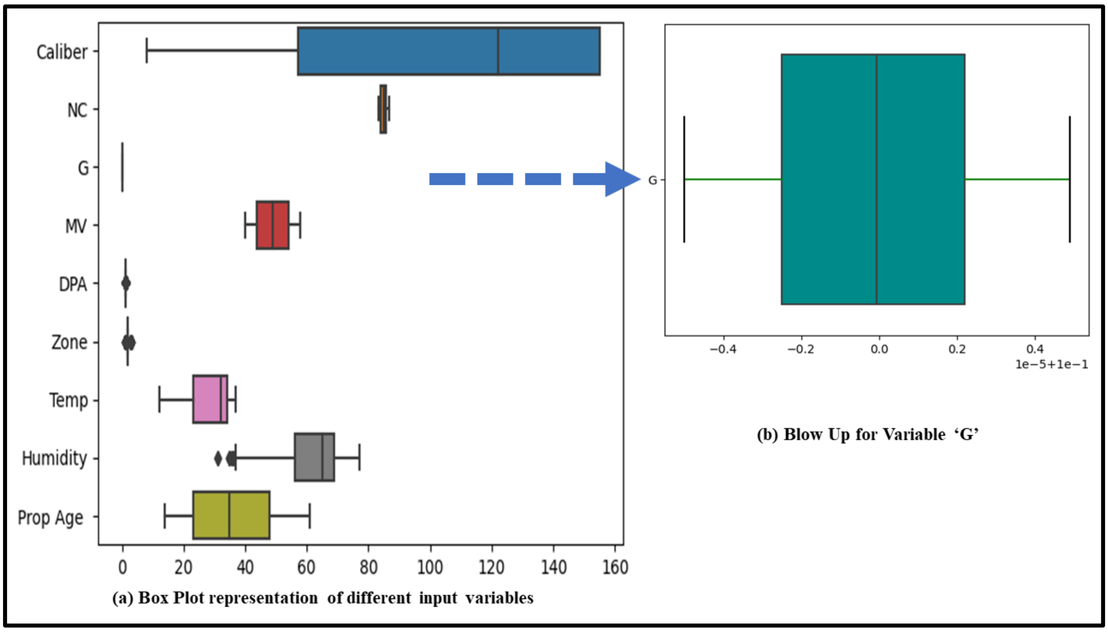

Figure 8: Box plot showing data distribution of input variables for RES prediction.

The **figure 8** shows box plot presentation for different input variables including C, NC, G, MV, DPA, zone, temperature, humidity and prop age, whereas figure 5 (b) is a blow up of variable 'G'.

5.2 Preprocessing and Feature Selection

A relevant subset of features or variables to be used in a predictive model are found via the feature-selection technique. This is a key step since it helps the model become more efficient, reduces over-fitting, and ultimately improves its capacity to generalize. The best features are selected using a variety of ways, including filtering, wrapping, and embedded methods. The two most popular methods for ML applications, wrapper-based and filter methods, are best suited for addressing feature selection [75, 76].

Wrapper approaches employ an ML model to assess the efficacy of feature subsets. Forward selection, backward elimination, and recursive feature elimination are a few examples of typical wrapper approaches. By optimizing a distinct objective function that gauges the effectiveness of the model, a subset of characteristics is chosen [77].

It is best to use input parameters that have been shown to affect the model's outcomes in order to ensure maximum model efficiency. Some input features had low R2 scores and high RMSE values, but they were left in since it was thought that even if they might seem unimportant, they still provide some context for the ML model. [78-80]. The primary purpose of feature selection is to identify a set of input variables that can faithfully represent the input data, limit the impact of noise or irrelevant elements, and generate accurate prediction results [75, 81].

When using a filter method, the relationship between the features and the desired outcome is investigated, each feature's importance is assessed, and only the most important features are kept. This makes it easier to exclude features from subsequent analysis that are redundant or irrelevant. The Chi-Square, mutual information, and correlation coefficient are a few illustrations of common filtering techniques. These are helpful for highlighting key aspects to be focused upon [81]. Hybrids of the filter and wrapper methods were used to select features.

Each data set contains both the output (RES%) and the input parameters. The initial composition, ambient and storage conditions, and propellant age were among the seventeen input characteristics chosen for this study, with RES% serving as the output parameter.

Table 2: GA based features selected.

Model Type	Feature Selected for GA
SVM	C, Manufacturing Year, NC, DNT, M, H MV, DPA, Zone, T, Humidity
GPR	C, NC, DNT, M, H, DPA, T, Humidity, Propellant Age
Ensembled Tree	C, NC, DNT, G, M, H, MV, DPA, Zone, T, Humidity, Propellant Age
Regression Tree	C, Manufacturing Year, NC, G, M, H, DPA, Zone, T, Humidity, Propellant Age

5.3 Performance Evaluation Criteria

R2 (R-Squared) and RMSE (Root mean squared error), are two critical metrics used to evaluate predictive models. These variables are used to assess a model's predictive power [82]. Regression analysis relies heavily on the R-squared statistic, which enables us to determine the volatility in the dependent variable can be attributed to the independent variables. With a scale that ranges from 0 to 1, higher numbers indicate a more optimal fit between the model and the data. As such, R2 proves valuable for comparing the performance of multiple models on the same dataset [83, 84].

RMSE is a metric that quantifies the discrepancy between the anticipated and factual data of a model. The RMSE is helpful for comparing the effectiveness of various models and determining the extent of their errors [85]. It is well acknowledged that models with greater R2 and lower RMSE values function more accurately and predictably. There is no single "correct" value for either metric [86]. This work increases our understanding of the various factors that influence aging and how those factors interact. This study is noteworthy because it combines four ML techniques with a GA strategy for feature selection and ML model hyperparameter tuning. To ascertain the impact of input parameters on the output variable, we conducted analyses of feature importance and partial dependence. Furthermore, a correlation plot was utilized to scrutinize the interrelationships among different variables [87]. ML will provide a comprehensive and unique understanding towards insights into the serviceability of propellants.

The effectiveness of the regression models was evaluated using coefficient of determination (R2) and RMSE. Training (80%) and testing (20%) subsets of the data were created, and the default hyperparameters in the MATLAB toolbox were used for the preprocessing of GPR, ET, RT, and SVM [88]. The 5-fold cross-validation method was employed in order to prevent overfitting and data loss. The GA was used to optimize the hyperparameter values after obtaining them from the regression model toolbox. Optimized hyperparameters were used to build and evaluate the regression models. The R2 and RMSE were calculated using the following formulas, which are often used in statistical analysis to assess the quality of fit of a regression model.

$$RMSE = \sqrt{\sum_{i=1}^{N} (x_i - \hat{x}_i)^2 / N} \,,$$

$$R^2 = 1 - \sum_{i=1}^{n} (\hat{y}_i - y_i)^2 / \sum_{i=1}^{n} (y_i - \overline{y}_i)^2$$

5.4 Optimization of ML methods

For this investigation, a regression learner program for MATLAB's machine learning models was used. Following the selection of each model's tuning parameters from the toolbox, the 5-fold cross validation and real standardized data were kept. Data must be altered to have a mean of 0 and a variance of 1 to be standardized. This is a standard approach in machine learning to guarantee that all features are scored on the same scale and given the same weight in the model.

A technique for assessing a model's performance is the 5-fold cross-validation. Utilizing 5-fold cross-validation was the better choice because it will lessen the variance of the performance estimate given our smaller dataset. Bias and variance are two sources of error in machine learning models. A model with small variance and little bias should be sought for. This is known as the bias-variance trade-off [89]. The dataset was trained using four different models: GPR, SVM, ET, and RT and was optimized using GA. The values of the hyperparameters obtained by GA are shown in **Table 3**. SVM optimized variables were: standardize data: true, box constraint: 4.8614, kernel scale: 2.1399, epsilon: 0.056476, and kernel function: gaussian. Similarly for ET, parameter values for GA were ensemble method: bag, number of learners: 135 and minimum leaf size: 1.

Table 3: Parameters Selected: Ranges and Optimized Values

ML Method	Parameters	Ranges	Optimized Values
SVM	Box constraint Kernel scale Epsilon Kernel function Standardize	0.001-1000 0.001-1000 0.00016308-16.3084 Gaussian, Linear, Quadratic, Cubic True, False	4.8614 2.1399 0.056476 Gaussian True
GPR	Sigma Kernel function Basis function Kernel scale:	0.0001-1.9371 Nonisotropic Exponential, Nonisotropic Matern 5/2, Nonisotropic RationalIsotropic Exponential, Isotropic Matern 3/2, Isotropic Matern 5/2, Isotropic Rational Quadratic Constant, Zero, Linear 0.147-147	0.00031766 Nonisotropic Matern 5/2 Zero 0.22918
Ensembled Tree	Ensemble method Number of learners Minimum leaf size Number of predictors to sample	Bag, LSBoost 10-500 1-149 1-17	Bag 135 1 15
Regression Tree	Minimum leaf size	1-149	6

5.5 Prediction Performance

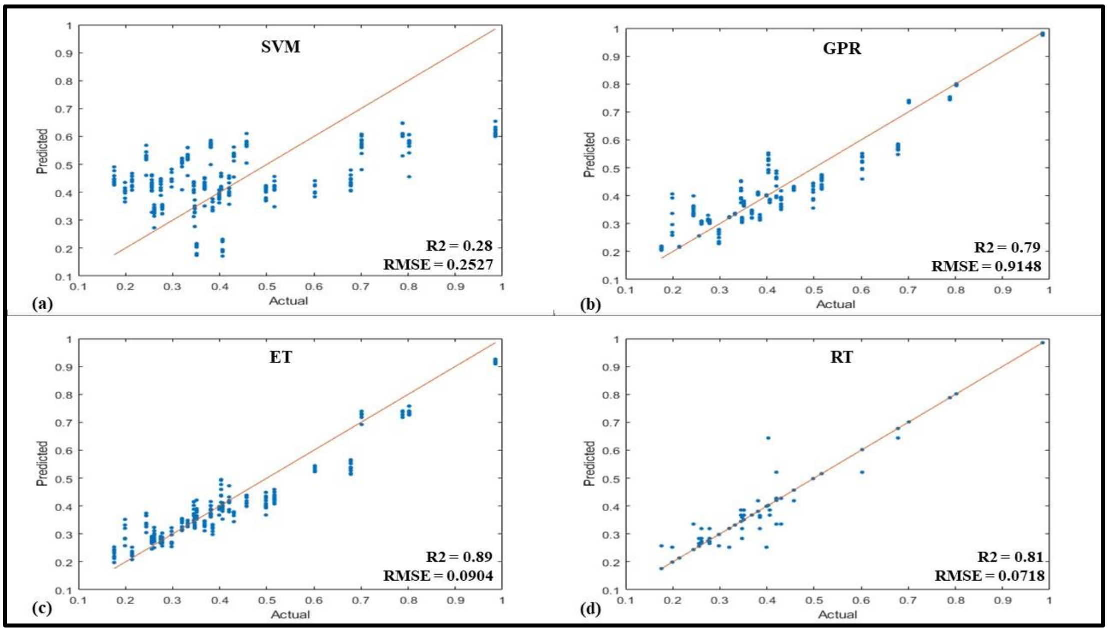

Figure 9: Comparison of different ML models for RES % (a) SVM (b) GPR (c) ET and (d) RT.

SVM, GPR, ET, and RT as ML models are employed for RES % prediction. Before features were chosen, ET's R^2 and RMSE values were 0.78 and 0.8454. The value of R^2 for the ET model was attained at 0.89 after employing the GA-based feature and optimized hyperparameters, and the RMSE was calculated to be 0.0904. The performance of ET-GA based model was found to be more acceptable as compared to SVM, RT and GPR for prediction of RES (**figure 9).**

Table 4: R2 and RMSE comparison for building and testing models.

Model	Initial R^2	Initial RMSE	Training R^2	Training RMSE	Testing R^2	Testing RMSE
SVM	0.23	0.8454	0.28	0.2527	0.18	0.1198
GPR	0.71	0.9385	0.79	0.9148	0.81	0.3797
ET	0.78	0.8454	0.89	0.0904	0.85	0.0198
RT	0.74	0.9319	0.81	0.0718	0.80	0.2102

Table 4 shows the R^2 and RMSE values for SVM, GPR, ET, and RT during training and testing. Both R^2 and RMSE were used as evaluation criteria for the best model and

their values were compared. Results obtained by running the GA based feature section on SVM model were not found to be satisfactory. From table 4 it was found that ET model best fit the performance evaluation criteria followed by RT and GPR.

5.6 Features Importance.

Table 2 depicts the features selected for prediction of RES % once each model was coupled with GA. To assess the importance of each selected feature, we used shapley method. Shapley values for machine learning models can be calculated using the "shapley" function in MATLAB's Statistics and Machine Learning Toolbox. This function creates a "shapley" object for a machine learning model using the query point by computing the shapley values for all features for the provided query point. These numbers describe how specific features affect a prediction at the given query point.

Our GA based model predicts the relation between RES % value, on which aging and serviceability of SBP is dependent, and factors like initial composition, temperature, humidity, age of propellant, manufacturing year and temperature zones in which propellants were stored. The comparison of input parameters was assessed using the ET-GA model. **Figure 10** shows that propellant age, temperature, humidity, Zone and DPA had a significant effect on the RES value, compared to initial composition, which have a minimal effect. This effect is likely due the reason that mass % of different of materials used in manufacturing SBPs is kept constant. It was also recorded that caliber propellant lot used as sample has a minimum effect mainly due to the fact all sample were from the same caliber having similar composition and propellant shape.

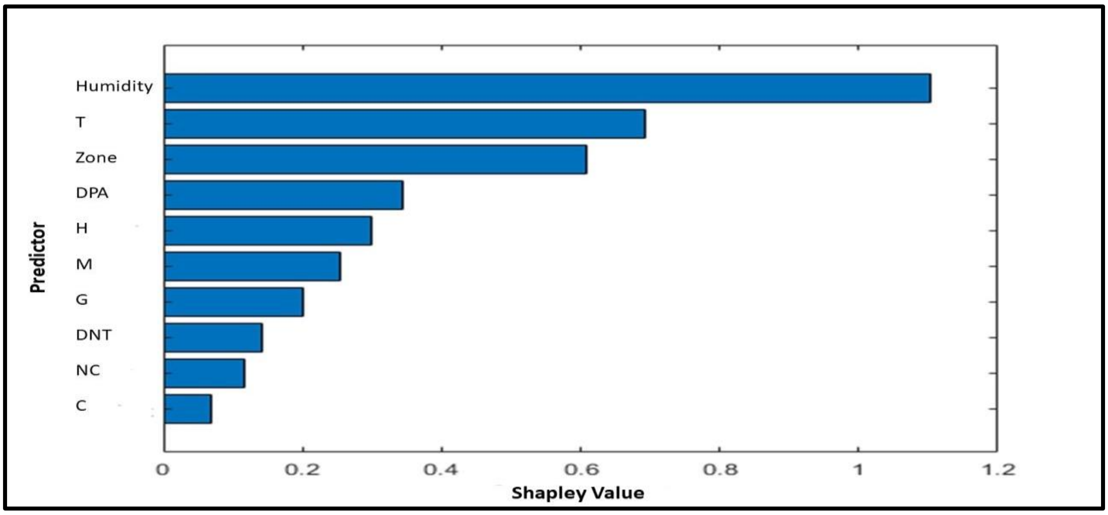

Figure 10: Feature importance in predicting RES (%)

5.7 Partial Dependence Analysis (PDA)

In order to evaluate the influence of input features on predicted outcome of a machine learning model, MATLAB leverages partial dependence plots (PDPs). These plots also have the ability to detect non-linear associations between input features and predicted outcomes, as well as interactions among input features [90, 91].

Using ET with GA, PDPs were created for the selected features. These plots are shown in **figure 11**. The correlation between RES and temperature and humidity is depicted in **figure 11(b)**. A drop in RES % is evident with rising temperature. **Figure 11(a)** illustrates the impact of initial DPA% and temperature. For our collected data, the storage temperature is in the range of 10 to 35 ^{o}C. It is observed that increasing temperature decreases RES (%) value.

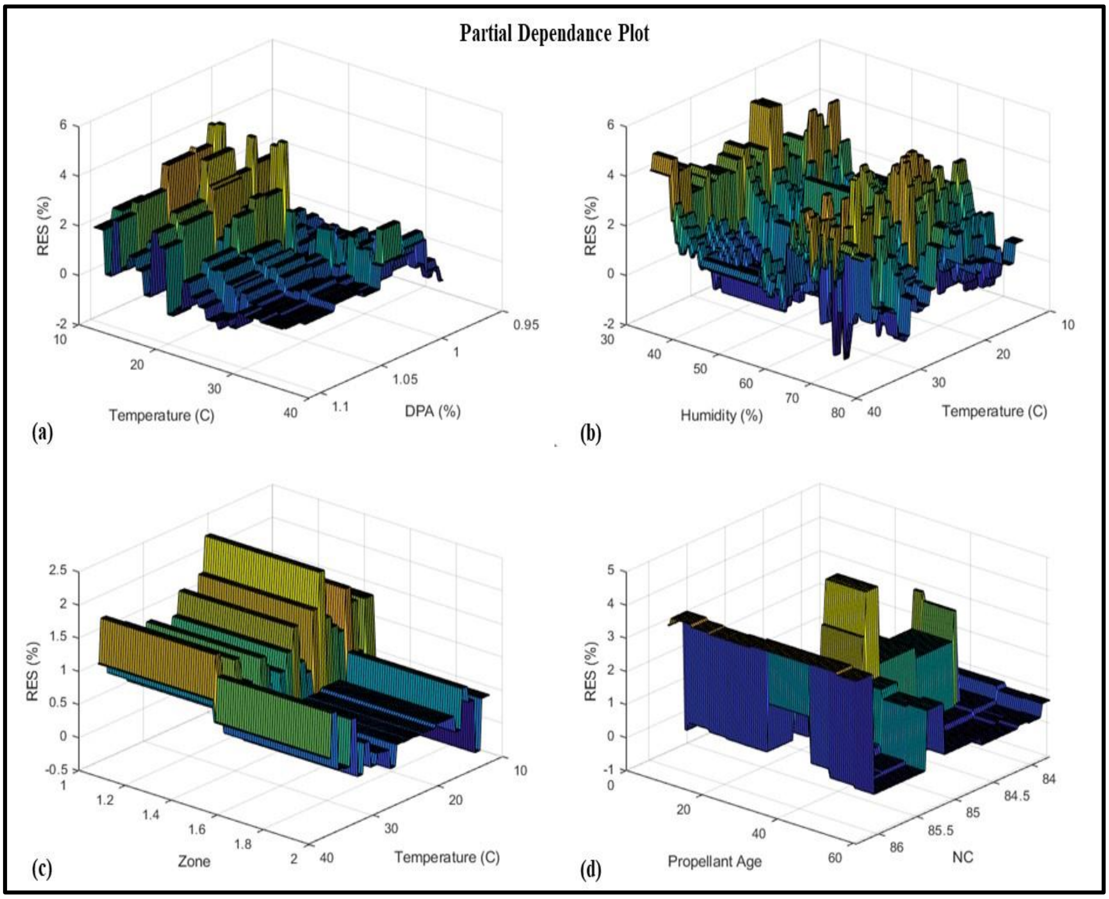

Figure 11: Partial dependence plot of ELT-GA model.

5.8 Pearson Correlation Plot

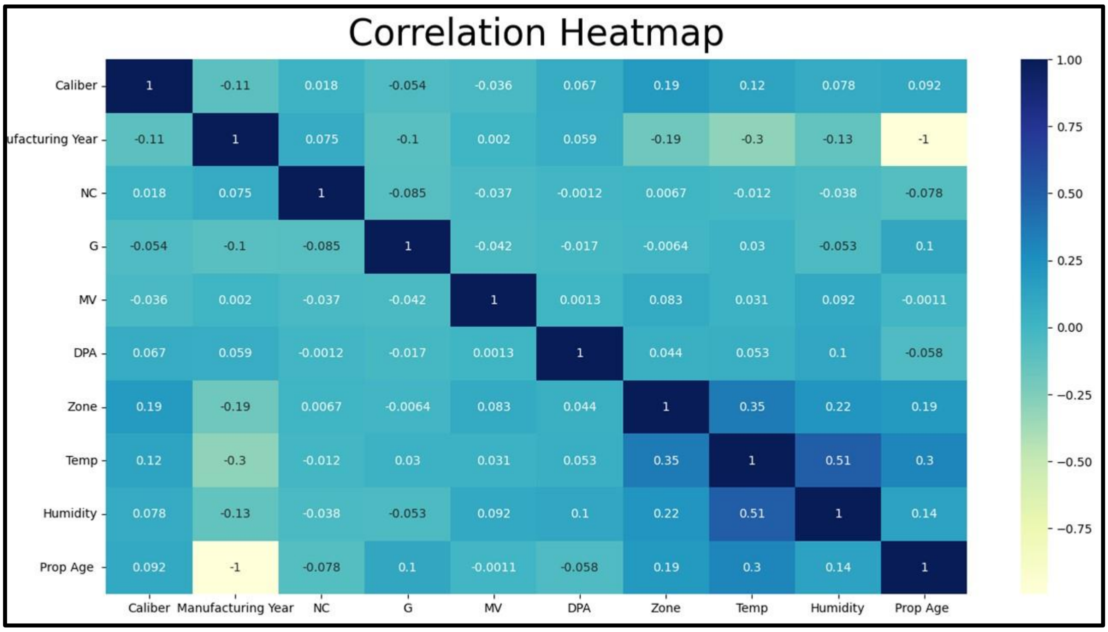

Figure 12: Correlation matrix plot showing Pearson's correlation coefficient between variables.

Pearson correlation heatmap is a graphical representation of the Pearson correlation coefficients as given in figure 12 between multiple variables. By utilizing this approach, it is possible to visually represent the intensity and orientation of the linear associations between two groups of variables. The correlation values are represented by colors on the heatmap, with one hue designating positive correlations and another negative correlation. The color's saturation reveals how strong the correlation is. The selection of features and an understanding of the data's structure can both be aided by the usage of Pearson correlation heatmaps, which are effective for seeing patterns and interactions between several variables [92]. A strong correlation suggests that as one measure rises, the other should rise as well. From **figure 12**, relation of temperature and humidity with PCC value of 0.51 effect the DPA percentage. When two variables have a negative correlation, one variable rises while the other one declines, for example the PCC value of DPA and NC percentage.

5.9 Validation of Prediction using HPLC Analysis

Due to its exceptional ability to provide higher resolution and increased sensitivity as compared to alternative approaches, the use of HPLC has gained substantial importance as a chromatography technique [93]. The validation of the meticulously developed predictive framework was a crucial step in the process of creating a comprehensive ET-GA based prediction model. HPLC analysis became an essential tool for completing this validation. In order to assess the viability and functionality of SBPs based on predetermined benchmarks outlined in STANAG 4620 and AOP-48 [26, 37] RES% was taken for the samples whose data has been used for model. The experimental RES% values obtained through HPLC analysis and the anticipated values produced by the constructed model were compared for this validation.

During the model validation process, three separate sample datasets were used as inputs to the prediction model. The model's resulting projected outcomes were compared to the corresponding values obtained through careful HPLC examination. The results of this careful comparison showed a mere 5% error margin (table 5), demonstrating the predictive model's remarkable accuracy and precision in estimating RES%. The implications of these findings go beyond simple statistical validation; they highlight the predictive model's effectiveness in not only accurately quantifying RES% but also in making wise judgments about the operational integrity of propellants in accordance with the specified standards.

In conclusion, the focus of the current study was the development and validation of an ET-GA based predictive model, a task that required the use of HPLC analysis to determine the RES%.

Table 5: Comparison of Actual and Predicted Values

Sample	Predicted RES %	Actual RES % using HPLC	% error
1	0.403	0.415	2%
2	0.613	0.648	5%
3	0.402	0.385	5%

5.10 Graphical User Interface

A straightforward app or Graphical User Interfaces (GUI) was created using MATLAB. By removing the need for users to learn a language or submit commands to utilize the application, these apps provide point-and-click management. With the help of a GUI, users may build interactive graphical programs that include buttons, sliders, menus, and other graphical elements. These GUIs offer a simple and clear user interface for manipulating, analyzing, and visualizing data. Users can build unique interfaces for their programs using MATLAB's GUI creation tools without having to have extensive programming knowledge. Using drag-and-drop features, they can quickly design and arrange components, establish characteristics and behaviors, and create code to give the components more functionality. In the end, MATLAB's GUI offers a simple method to build interactive visualizations of complex data, making it particularly helpful for researchers and engineers that work with enormous datasets.

There are three different approaches to develop a GUI in MATLAB; the interactive app designer was chosen for this paper to lay out the visual elements and program the app's behavior. It enables to switch between writing code in the MATLAB editor and visual design on the canvas quickly.

The model prediction function employed by the GUI, the screen shot is given in **figure 13,** in this study will help us predict the RES%. The GUI produced as part of this research will assist researchers to simply enter in initial composition, storage temperature, humidity, and age of propellant. Using the criteria outlined in STANAG 4620 and AOP-48, the app will carry out sentencing of propellant [26, 37].

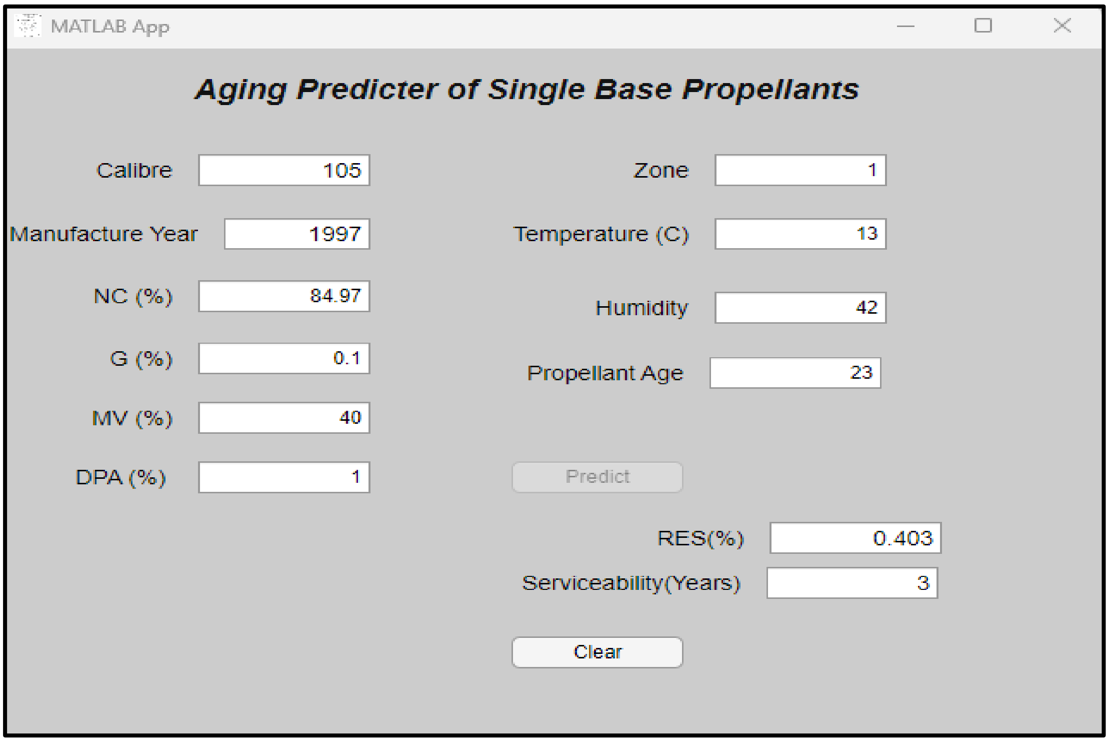

Figure 13: Screen Shot of GUI Developed for Prediction of Serviceability of Propellants.

Conclusion

In conclusion, this study demonstrated the effectiveness of using ML models in combination with GA for predicting the aging of SBPs. By analyzing various variables such as initial composition, temperature, relative humidity, and moisture content, the study provided insights into the aging process and its impact on propellant functionality. The use of predictive ML models and GA optimization also allowed for the automation and optimization of surveillance techniques. Overall, this research provides a practical solution to enhance the efficiency and reliability of SBP surveillance and testing methods. Future research could also benefit from this study by expanding the analysis to double- and triple-base propellants. Possible ways to reduce the percentage error between predicted RES and measured RES by HPLC analysis include improving the accuracy of the HPLC instrument calibration, ensuring precise and consistent data collection and input, and reducing human error during HPLC analysis. Additionally, incorporating additional data points and increasing the sample size may improve predictive models, ultimately leading to more accurate predictions of aging and serviceability of SBPs.

Future Recommendations

- To improve the precision of aging prediction models, particle swarm optimization (PSO) and GA can be used together.
- The predictive machine learning model developed has the potential to be used in aging prediction for double and triple base propellants. Despite having different chemical composition, they also undergo aging that can affect their stability and performance.
- Extensive testing over long periods of time is frequently needed for traditional techniques of evaluating propellant aging. By employing the model at industrial scale this predictive model might considerably minimize the time and cost involved with such testing.

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