New Design Method of Solid Propellant Grain Using Machine Learning

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Abstract: The correlation between solid propellant grain configuration and burning surface area profile is a complicated nonlinear problem. Nonlinear optimization has been adopted to design grain configurations that satisfied the objective area profiles. However, as conventional design methods are impractical with limited performance, it is necessary to investigate alternatives. Useful information for grain design can be obtained by analyzing the aforementioned correlation. However, this aspect has not been studied owing to the requirement of large amounts of data and analysis techniques. In this study, machine learning was used to develop a new design method. The objective of machine learning was to train a model to classify classes of data. The database stores various sets of configuration variables and their classes. The proposed Gaussian kernel-based support vector machine model predicts the class of newly designed grains. The results verified that the model accurately predicted the class of the set of configuration variables and can be used to modify the set of configuration variables to satisfy the requirement. Thus, it was confirmed that machine learning is an appropriate approach to grain design; however, further research is needed to analyze its practicality.

Keywords: solid rocket motor; grain design; machine learning; support vector machine

1. Introduction

Solid propulsion systems can generate strong forces within an extremely short time after ignition; however, controlling the thrust is challenging. Therefore, it is necessary to design a suitable propellant grain configuration. Grain design involves the process of obtaining a set of configuration variables that can satisfy the desired burning surface area profile with burning time, which is referred to as burn-back analysis. Each configuration variable affects the area profile, and it is difficult to predict changes to the area profile because of the complicated effects of the modified variables [1]. Therefore, sufficient design experience is required and a redesign, based on the existing data, is necessary to modify the configuration variables to obtain the area profile [2]. However, because the correlation between the configuration variable and the area profile is not clearly identified, it is difficult to modify the configuration variable; this significantly impedes solid propellant grain design.

Previous studies have mainly addressed this problem by applying optimization techniques rather than correlation analysis [1–3]. However, because grain design is a multi-variable nonlinear problem, it is extremely difficult to achieve an optimum design. Optimization techniques are divided into deterministic and stochastic methods [4], based on whether the method incorporates probabilistic factors. The deterministic method has good search performance for the optimum solution but easily converges on the local solution. The stochastic method exhibits high performance for global solutions but has difficulty converging to an optimum solution. Optimum grain design requires the advantages of both methods. Nisar and Guozhu used deterministic methods to design wagon wheel geometries [3], and Kamran used stochastic methods to design cylinder and star geometries [5]. However, the single optimization technique is impractical because of the disadvantages...
associated with each method. To overcome this problem, a hybrid optimization technique that links two optimization techniques was studied. Raza and Liang used two stochastic methods to design wagon wheel grains [6] and Oh et al. confirmed that stochastic and deterministic methods can be combined to utilize the strengths of both techniques [1]. However, hybrid optimization techniques also lack universality and flexibility. Recent studies consider hyper-heuristic optimization [7], which uses various optimization techniques; the most feasible result is to use a new starting point for these techniques. As research progresses, the possibility of developing an optimum design that satisfies the requirements has increased. However, considering the time and cost of using multi-optimization techniques, this is not practical.

Another issue that requires investigation is utilizing stored data. Solid propulsion systems have been designed in various configurations for decades. Usually, defense research institutes or companies possess large amounts of design and experimental data. However, the optimum design study does not use stored data directly because it includes a burn-back analysis process. Large amounts of new data generated during the optimization process are stored but are not used in the subsequent design.

The saved data contained correlations between the configuration variables and the area profile. Using these correlations, grain design can be performed easily and directly. Currently, general grain design involves a stochastic approach—similar to the genetic algorithm—that randomly generates a set of configuration variables and uses the most suitable result. If the research proceeds successfully, a design model that directly calculates the feasible set of configuration variables would be developed. Despite these advantages, the correlation has not been studied because grain design is a nonlinear problem; as such, analysis is extremely difficult because each configuration variable has a complicated effect on the area profile.

Machine learning is a useful technique that can address this type. This technique is used in a variety of fields because it can obtain meaningful information from stored data [8,9]. However, no study has thus far been performed on grain design. Therefore, in this study, a fundamental investigation of grain design using machine learning was conducted. The goal of this study was to apply and validate machine learning instead of a burn-back analysis in the design process. The classification method and optimization techniques were applied to obtain the configuration variables with a neutral area profile for a star grain, which is generally used as a solid propellant [10]. The database including a set of configuration variables and area profiles was constructed to be used for machine learning. Classes were designated as satisfying the design objectives (Class 1) and others (Class −1). Support vector machine (SVM) is applied as a machine learning method that can learn complicated boundaries, and the Gaussian kernel-based SVM is adopted to classify the class. The machine learning-based design method is confirmed as suitable for grain configuration design.

2. Grain Optimum Design

2.1. Optimum Design Process

The optimum design involves three steps, as shown in Figure 1 [1]. The first step is grain design. This is the process of obtaining a set of configuration variables suitable for the objective and a new set is created to better meet the requirements using design experience or an optimization technique. The second step is the process of obtaining the area profile of the designed grain, which requires fast and accurate analysis technology owing to the large calculation cost. This is the grain burn-back analysis step. The third step is to assess objective levels. If the level does not satisfy the requirement, the grain will be redesigned.

The optimization technique corresponding to the first step was the main target of previous studies. The set of configuration variables determines the initial grain configuration, and the initial configuration determines the area profile. Therefore, a correlation exists between the configuration variable and the area profile. However, because the influence of each configuration variable on the area profile is complicated, the correlation cannot be
easily understood. Therefore, the optimum grain design is classified as a multivariable nonlinear optimization problem.

The third step is to define the objective of the optimum design. For a grain with a neutral burning surface area profile, the standard deviation can be used to define the objective. The difference between the average surface area ($A_m$) of the grain and the grain burn-back analysis result ($A_n$) was calculated at 0.01 mm intervals and the dimensionless standard deviation ($\sigma$) was obtained using Equation (1). The smaller the size of the standard deviation, the closer is the area profile to the neutral profile, and when a grain configuration smaller than the objective standard deviation is designed, the grain design is considered complete. Figure 2 and Table 1 present the configuration variables of the star grain.

$$\sigma = \sqrt{\frac{(A_1 - A_m)^2}{A_m^2} + \frac{(A_2 - A_m)^2}{A_m^2} + \cdots + \frac{(A_n - A_m)^2}{A_m^2}}$$

(1)

Figure 2. Star grain configuration.

Table 1. Star grain configuration variables.

| Symbol | Configuration Variable          |
|--------|---------------------------------|
| N      | Number of star branches         |
| Re     | External radius (mm)            |
| Ri     | Internal radius (mm)            |
| w      | Web thickness (mm)              |
| f      | Fillet radius (mm)              |
| e      | Angle coefficient               |

2.2. Grain Burn-Back Analysis Technique

In the second step, burn-back analysis is the process of determining an area profile. In the conventional process, the area profile is calculated by entering the configuration variables generated by the optimization technique into the grain-burn-back analysis. Grain burn-back analysis techniques can be classified into three types. The simplest technique is
the analytical method [11,12], which analyzes the structure of the lines and surfaces that constitute the grain configuration. The analysis result is obtained via equations that can calculate the line and area [11]. Because analytical methods use equations, the surface area can be immediately obtained. However, the analysis of complicated configurations is extremely difficult; thus, limited 2-D configurations are usually analyzed using this technique. The drafting method uses a computer-aided design (CAD) program [10,13]. CAD can create and edit 3-D configurations and can also measure the area. It can be used to analyze the burning surface area of complicated 3-D grains. However, this method requires considerable time and manpower, or a complicated macro. The numerical method discretizes the grain configuration and analyzes the motion of the surface [14,15]. This method stores surface position information in a 3-D coordinate system. The burning surface area is analyzed by updating the position information in the numerical method. This method is not suitable for optimum design because it requires the most computation time among the three types.

2.3. Necessity for New Grain Design

Grain burn-back analysis should be executed rapidly because large amounts of grain configurations are generated during the optimum design process. Therefore, a previous study used an analytical method, and the optimum design target was limited to configurations that could be geometrically analyzed, such as slots and stars. It is necessary to use a different burn-back analysis method for optimizing the design of the complicated 3-D configurations used in propulsion systems. However, because automation is difficult with a long burn-back analysis time, it is difficult to apply the existing optimal design process. In this regard, this study developed a new grain design method and confirmed its feasibility.

Machine learning can acquire meaningful information from data. If the correlation between the configuration variable and area profile can be learned using machine learning, the performance of the newly designed grain can be predicted with high accuracy. Figure 3 shows the grain design process using machine learning. The database consists of stored data, such as a set of configuration variables and classes. A large amount of information is organized into databases and high-quality information is obtained through data mining; machine learning is then used to identify and evaluate meaningful patterns. The model is the result of machine learning and it calculates the margin of a set of configuration variables. The margin predicts the class of a set of configuration variables.

This study was conducted to determine whether machine learning is an appropriate method for grain design. The goal of grain design was to obtain a neutral burning surface area profile, which is called briefly the neutral profile in this study. The neutral profile was defined as having a standard deviation of ≤0.5. Class 1 was neutral and Class −1 was non-neutral, as listed in Table 2.

Table 2. Class classification.

| Class | Classification |
|-------|----------------|
| 1     | $\sigma < 0.5$ |
| −1    | $0.5 < \sigma < 1.0$ |

This study had two goals. The first was to create a model that can predict whether it is neutral. By creating a classification model from the saved data, we can verify whether the area profile is neutral without performing a burn-back analysis. Another goal was to modify the non-neutral shape to a neutral shape using the model. When the grain shape designed in consideration of various conditions is a non-neutral type, it is necessary to change it to a neutral-type through as few variable changes as possible. The database was constructed and a classification model was created using data mining and SVM. After checking the accuracy of the classification model, an arbitrary set of configuration variables was modified to a neutral configuration by using an optimization technique.
Figure 3. Grain design process applying machine learning (a) machine learning (b) design using model.

3. Machine Learning

3.1. Machine Learning

Machine learning refers to the recognition of complex patterns based on data or learning to make intelligent decisions. It is used in various fields as it can obtain meaningful information for satisfying specific purposes by analyzing a large amount of information; this is not feasible using human resources [8,9]. Machine learning needs a database. A database construction plan was established in this study, as specified in Table 3. Acquiring a large amount of data results in considerably useful sample data but is impractical as it also increases the construction time. In this study, the number of branches was fixed at five and the number of each variable was controlled to generate 49,500 sample data.

Table 3. Database construction plan.

| Configuration Variables | Design Range | Count |
|-------------------------|--------------|-------|
| N                       | 5            | 1     |
| Re                      | 100–200      | 11    |
| Ri                      | 5–50         | 10    |
| w                       | 5–50         | 10    |
| f                       | 2–10         | 5     |
| e                       | 0.1–0.9      | 9     |
|                         | Amount of stored data | 49,500 |

Machine learning requires the use of a suitable method for databases. The database has a label (class) of all inputs (the set of configuration variables), and the classes are 1 and −1. Therefore, it is a classification problem [8], and the SVM, which is known to have high performance in analyzing complicated interfaces of multiple variables [16,17], is adopted as an appropriate method in this study. In fact, SVM has been used in several prior studies owing to its ability to classify normal and faulty operation and predicted where the fault occurred [18–20].
3.2. Support Vector Machine (SVM)

The SVM learns the sample data and defines the boundary between classes, which is called a hyperplane. The classification model can predict the class of a new input variable using a hyperplane. Figure 4 shows an example of a linear SVM. The data points have coordinates ([x₁, x₂]) and class (y). In SVM, data is defined as a vector, as shown in Equation (2).

\[(x_1, x_2, \cdots, x_n, y)\]  

(2)

A margin is the dot product of the hyperplane and data. The SVM calculates the hyperplane vector \(w\) and constant \(b\) where all data satisfy Equation (3) [16]. The margin of the support vector is 1.

\[y \times (w \cdot [x_1, x_2, \cdots, x_n] - b) \geq 1\]  

(3)

The class of new points can be predicted using the margin. The positive margin is Class 1 and the negative margin is Class -1. For example, the new point A in Figure 4 is classified as Class -1 by the hyperplane.

The grain design requires a nonlinear SVM because changes in the configuration variable have complicated effects. Nonlinear SVM generally uses kernel functions to define the hyperplane. In this study, nonlinear SVM was performed using a Gaussian kernel function [16]. The Gaussian kernel is a representative kernel of the SVM and is a suitable method for learning a complicated boundary.

3.3. Gaussian Kernel

In the Gaussian kernel, \(C\) and \(\gamma\) are important variables in SVM that determine the hyperplane. \(C\) determines the range of the support vectors used in hyperplane learning. When \(C\) is large, the range narrows, and the number of support vectors decreases. \(\gamma\) determines the effect of the support vector on the hyperplane. When \(\gamma\) is small, the hyperplane is significantly affected by the support vector and the shape of the hyperplane changes rapidly. Using small \(C\) and \(\gamma\) produces a complex and fine hyperplane; however, it is prone to overfitting. Conversely, using large values of \(C\) and \(\gamma\) ignores the fine boundary shape and learns a coarse hyperplane, which is prone to underfitting. The error can be reduced by using suitable \(C\) and \(\gamma\). The effects of \(\gamma\) and \(C\) on the hyperplane are described in detail in Reference [16]. SVM is built in various free and commercial software [21]. MATLAB R2019b was used for this study. MATLAB includes machine learning and a
variety of kernel functions. To optimize C and \( \gamma \), Bayesian optimization techniques in MATLAB are adopted in this study.

The Gaussian kernel is because the margin exhibits a Gaussian distribution. The margin changes rapidly around the support vector and is constant in the region far from the support vector. The main factor that makes optimal grain design difficult is the local solution. If the characteristics of the margin can be applied, the optimization problem can be easily solved.

The Styblinski–Tang function was used to determine the effect of the margin on the optimization problem. This function is Equation (4), which is an optimization performance test.

\[
f(x_1, x_2) = Z = \frac{1}{2} \sum_{i=1}^{2} \left( x_i^4 - 16x_i^2 + 5x_i \right)
\]

Criteria were set to classify local and optimum solutions and a Gaussian SVM was used. Figure 5 shows the contour of the Styblinski–Tang function. The Z contour has three local solutions and one optimum solution but the margin contour does not have a local solution. Figure 6 shows the difference between Z and the margin. Figure 6a compares the classification criteria and the hyperplane. The shapes of the two lines are almost the same but the difference between the two lines is found in the magnified figure. The factors that cause the difference can be verified in Figure 6b. In the enlarged figure, the SVM only considers the class and the hyperplane is the middle of the two support vectors. However, the criterion was close to that of class \(-1\). Because of this difference, it is possible to misclassify the class near the hyperplane. The sample data should be analyzed to avoid errors. The sample data of Class 1 has a positive margin. In this example, the smallest margin of the sample data for Class 1 is 0.1. Therefore, if new data has a margin greater than 0.1, they are clearly class 1. The unique part in Figure 6b is the local solution. Z has the optimum and local solution but the margin eliminates the local solution because it only changes around the sample data. This is a useful effect that reduces the difficulty of the search process.

![Styblinski–Tang function](image)

(a) Z contour (b) Margin contour.

Figure 5. Styblinski–Tang function (a) Z contour (b) Margin contour.
4. Analysis Results

4.1. Data Mining

The database contains not only the configuration with a neutral profile but also the progressive, regressive, and impossible combinations of configuration variables. To obtain useful information in the database, a set of configuration variables was mined using standard deviation, as shown in the class classification in Table 3 [22].

Through the data mining process, 11,524 Class 1 and 7564 samples Class −1 samples were classified. A total of 30,412 data were excluded. These data cannot improve classification accuracy and are impeding factors that increase the learning and classification time.

4.2. SVM Results

This study generated a classification model that can predict how satisfied the conditions with the neutral profile are, as presented in Table 4, using the Gaussian kernel SVM. Learning and validation were performed using all of the sample data. Bayesian optimization has been used to optimize C and \( \gamma \) [21] as mentioned in 3.3. \( C = 19.71 \) and \( \gamma = 0.43 \) were used to obtain a classification model with an error rate of 0%. To verify the overfitting, a hyperplane shape construction and classification test were performed.

| Axis | Range   | Count |
|------|---------|-------|
| \( x_1 \) | 5−5     | 101   |
| \( x_2 \) | 5−5     | 101   |

Figure 7 shows the margin contour of the external-internal radius. The blue dots are Class 1 sample data and the red dots are Class −1 sample data. From Figure 7, it can be confirmed that the hyperplane (red line with margin = 0) classifies the class appropriately. Learning was successful because overfitting did not occur and the hyperplane effectively classified the classes. The margins of the sample data of Class 1 were analyzed to avoid errors caused by the difference between the hyperplane and the margin. The smallest margin is 0.0106. Therefore, the neutral configuration design with a neutral profile ends when the margin is greater than 0.0106.
The class of cases was calculated to verify the model’s prediction performance. Table 5 lists the set of configuration variables and prediction results. Each case consisted of an arbitrary set of configuration variables that did not exist in the database. The model classified Cases 2 and 3 as Class 1. To verify the classification results, the standard deviations were calculated using burn-back analysis of the analytical method, as listed in Table 6. It was confirmed that the results of the grain-burn-back analysis and SVM model were the same. Through this, it was proven that the class prediction using the model was accurate and that the SVM learned the correlation between the configuration variables and the burning surface area profile.

**Table 5. Classification test results.**

| Case | 1 | 2 | 3 | 4 |
|------|---|---|---|---|
| Re   | 139 | 152 | 172 | 189 |
| Ri   | 26  | 43  | 24  | 16  |
| w    | 37  | 41  | 11  | 47  |
| f    | 7   | 2   | 10  | 3   |
| e    | 0.78 | 0.53 | 0.11 | 0.61 |
| Margin | −1.13 | 1.15 | 0.62 | −0.03 |
| Classification result | Non-neutral | Neutral | Neutral | Non-neutral |

**Table 6. Analytical method results.**

| Case | 1 | 2 | 3 | 4 |
|------|---|---|---|---|
| σ    | 0.87 | 0.08 | 0.41 | 1.43 |
| Class | −1 | 1 | 1 | −1 |
| Analysis result | Non-neutral | Neutral | Neutral | Non-neutral |
4.3. Grain Design Using SVM

Conventional design methods using standard deviations pose a risk to nonlinear global optimization problems with many local solutions. Therefore, a stochastic method is required that exhibits high global search performance but also requires considerable computational time. However, converting to a margin can reduce the time required for grain design because the design difficulty can be reduced. To confirm the usefulness of the SVM, the grain optimum design was performed by assuming a multidisciplinary design optimization (MDO) [23,24]. The star grain design with a neutral burning surface area profile was performed using arbitrary missions and structural design results. The grain design used the simplex method, which is a typical deterministic method [16,19]. This method searches for a set of configuration variables that are close to the optimum solution by modifying the initial configuration variables [21]. This method exhibits fast and accurate search performance and is used in various fields because it can solve nonlinear problems that use multiple variables [25,26]. However, when the initial value is not suitable, it converges to the local solution and, thus, the global search performance is low. Therefore, it is not suitable to only use this method in grain design, despite achieving a very fast solution. However, if a local solution that does not satisfy the requirement is eliminated, the simplex method can be a useful tool for grain design optimization.

To confirm whether machine learning is useful for grain design, grain design was performed under the condition that the simplex method failed, as presented in Table 7. Some of the shape parameters were determined during the MDO process and the constraints of the grain design were set. The requirement determines the operating time (web length) and the external radius is determined from the structure. The initial input value was the end of the variable range. This input value is a configuration with a non-neutral profile (Class −1).

Because the mass of the propellant is properly designed, the configuration change needs to be small. When using the conventional method, the grain design used the simplex method to search for a configuration with standard deviations less than 0.5. As a result of the search, the inner radius almost doubled and an abnormal filet radius was designed. This result shows the disadvantages of the simplex method, which does not apply a design range during the redesign process and converges to a local solution according to the gradient around the initial input value [27]. However, the simplex method with SVM has designed a set of configuration variables that satisfy a margin of more than 0.0106. The margin of the design results was 1.8, which corresponds to class 1. The standard deviation was 0.19 and it was verified that the class was correctly classified. Therefore, it was verified that SVM can reduce the difficulty of the search problem and conduct the design using the stored data.

| Configuration Variables | Constraints to Design | Initial Input Value | Optimization Results |
|--------------------------|-----------------------|---------------------|---------------------|
| Re                       | 182                   | -                   | -                   |
| Ri                       | -                     | 49                  | 95.18               |
| w                        | 44                    | -                   | 46.18               |
| f                        | -                     | 9                   | −9.33               |
| ϵ                        | -                     | 0.12                | 0.32                |

5. Conclusions

A fundamental study on grain design using machine learning was conducted. In this study, a new design method for machine learning was developed using stored data for grain design. The database for the burning surface area and configuration variables was constructed using analytic burn-back analysis and the standard deviation was calculated. The analysis results were defined as class 1 if it satisfied the requirement and class −1 if it did not. The SVM learned the condition that satisfied the requirements and obtained the classification model. This model separates the two classes using hyperplanes, enabling the
margin of the new set of configuration variables to be calculated. It was confirmed that the grain can be designed without additional analysis using the stored data. The classification model obtained via machine learning performed classification with high accuracy, verifying that it can replace burn-back analysis.

It was verified that machine learning is an effective method for optimizing grain design. Through this design process, it has been confirmed that the complicated effects of the configuration variables can be learned through machine learning and that the result is very useful. However, since the study was conducted at a fundamental level, there are some supplements. Although it satisfies the objective, it is necessary to perform an additional optimum design of the standard deviation. In the case of real grain design, there are various requirements—such as average area and burn time—but, in this study, only the standard deviation was learned and it is necessary to analyze whether the amount of sample data is adequate.

Further studies are required to develop a general method of grain design. Various topics were identified, such as the feasible size of the database, classification of multiple classes according to the average burning surface area, the use of multiple models for requirements, and training using randomly generated data. In a subsequent study, a practical grain design process has been considered and a study that will apply machine learning to the entire grain design process has been planned.

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