Detecting Transitions States in an Optical Emission Spectrum using Machine Learning

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ABSTRACT

Researchers are exploring ways of predicting and controling scramjet behaviors for usage in high speed engines. The present research seeks to use Optical Emission Spectroscopy (OES) sensors are now presented to predict these behaviors. This prediction requires the examination of the transition from one steady state to another. This research sought to use denoising techniques and machine learning algorithms to detect these transition in both simulated and real-generated spectra datasets. It was found that the algorithms and filters utilized generated between 97% and 98% detection accuracy.

CCS CONCEPTS

• Computing Methodologies → Machine Learning; **• Computing Methodologies-Modeling and Simulation**; **• Software and its Engineering** → Software Creation and Management;

KEYWORDS

Machine Learning, Denoising, Signal Processing, Support Vector Machine, Feedforward Neural Network

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1 INTRODUCTION

High-speed air-breathing engines are presently important in the fields of defense space exploration and transportation. This is because these engines (i) provide a higher specific impulse at a much lower weight profile than solid rocket motors and (ii) are capable of operating over longer ranges allowing for more operational flexibility. Presently Dual Mode Scramjets (DMSJ), which are engines that can be operated in both subsonic and supersonic combustion mode, are been investigated most promoted. Air-breathing engines however, tend to be more complex to operate than rocket motors because of the close coupling of the vehicle state with the engine performance and operability. With this comes the possibility of the breakdown of the supersonic airflow called the unstart [5]. The avoidance of unstart is of high priority but with scramjets it is hard to predict due to their sensitivity to pressure fluctuations within the system.

Researchers have looked at ways of predicting and controling scramjet behavior [10], however most methods utilize pressure measurements within the isolator and combustor to determine the shock location and the health of the combustion environment. The use of Optical Emission Spectroscopy (OES) sensors are now presented as an alternative in [5] as they can (i) decrease the phase lag of the control system and (ii) provide more information, as compared to pressure transducers, about the state of the combustion occurring within the engine by using chemiluminescence from emitting species [12]. These sensors could also be used in parallel with pressure sensors to enhance the total control performance of the system.

Improving the operability of DMSJs requires the measurement and analyzation of the spectral emissions data and the transition from one steady state to another. Each steady state effectively indicates the global equivalence ratio between distinct chemical species (OH and CH). The excited states (OH^* and CH^*) provide information such as the region of burned products and the region of initial fuel breakdown of DMSJs [8, 11] and are prevalent in combustion environments. A more relaxed species state is reflected by more light emission which is measured by the OES. Finding the distinction between the transition and steady states within transient OES data helps to determine where the transition occurs, thus enabling gain-scheduling in the OES controller which helps with DMSJ fuel control.

Capturing the chemiluminescence of species using streak cameras allows for measurement of light through imaging, although naturally generating photoelectrons. This method generates noise, which serves as an impediment to accurately identifying the transition state. Light penetrating the circumference of the camera is also characterized as noise which is not helpful during experimentation

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[11]. Denoising serves as an effective method of preprocessing the data for use in further classifying the various states, thus avoiding unfavorable trade offs such as a loss in time resolution through the use of other methods like averaging. Digital denoising filters such as Median filters, Savitzky-Golay filters, Wavelets and Moving Average filters enable a seamless and simple noise removal process. These filters can serve as mechanisms for efficiently classifying transient OES data because of their smoother signal frequencies which make outlining the transition point an easier task.

Research has already shown that OES can be used as an error signal in a combustion process for the purpose of control but did not actually incorporate the sensor into a control system [19]. This paper is based on research presently testing the use of OES sensors as a way of avoiding unstart. As such this paper seeks to examine data processing techniques to enhance sensing and control using data filtering and machine learning algorithms with the aim of classifying the transition state from the steady states and be able to identify when the transition occurs.

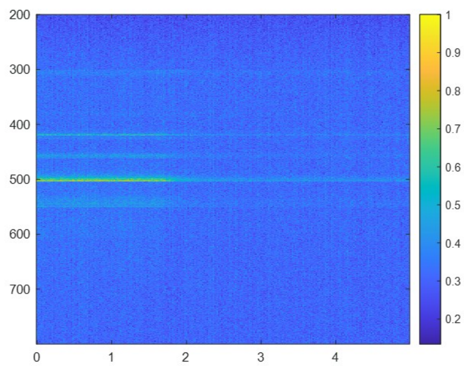

Figure 1: Sample Scramjet Transient Spectra

2 DATASETS

The ability to control DMSJs relies on sensing changes in the flowfield. The original emission spectra data did not provide successful responses or classification results.

Studying transient events from the scramjet emission spectra data (sample in Fig. 1) is necessary to understand the time scale and phenomena of events that can be measured and interpreted when relying on spectral emission measurements. The transient data received from this spectra shows transition from one steady state to another as seen in Fig. 3. From this the goal is to classify the transition state from the steady states and be able to identify when the transition occurs. This process would enable additional gain-scheduling in the controller, ideally resulting in a faster response and a ability to transition with smaller fuel step sizes using the OES Controller.

For this research there were two types of datasets collected - (i) real from the emission spectra collected from our partners at the University of Virginia Supersonic Combustion Facility (UVaSCF) and (ii) simulated ratio data (Fig. 2). Fig. 1 is the UVA spectra data, Fig. 6 and Fig. 7 show the UVA chemical OHCH ratio data calculated from the spectra. The goal of the research is to detect the transition stages from the chemical ratio sequences using the machine learning algorithms. To this end, we consider the supervised machine learning approaches where the labelled training data is built. In the simulated training dataset the duration of steady states and transition were randomly generated. Class 0 was defined as the two steady states while Class 1 was defined as the transition state from one steady state to another. $x_{0,i}(t) = base_{0,i} + n_0(t)$ denotes the observation data points in the steady states at time t where the noise is Gaussian $\mathbf{N}$ with zero-mean and covariance σ_0, that is, $n_0(t) \in \mathbf{N}(0, \sigma_0)$, $\sigma_0 = 0.008$ and $i = 1, 2$ for the two steady states. $x_1(t)$ denotes the data points in the transition period from the steady state with $base_{0,1}$ to another steady state with $base_{0,2}$, added by Gaussian noise $n_1(t) \in \mathbf{N}(0, \sigma_1)$, $\sigma_1 = 0.004$. If $base_{0,1} > base_{0,2}$, the transition is decreasing otherwise increasing.

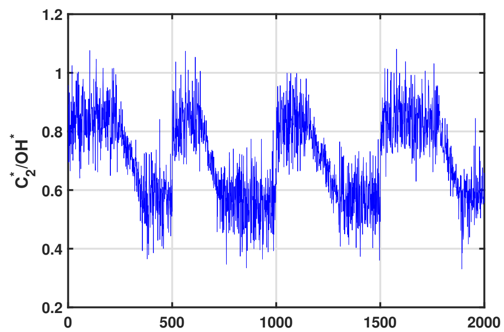

Figure 2: Simulated Raw Ratio Data: First 2,000 Samples

The training data included two types of transitions: one increasing transition and one decreasing transition. For each transition, there were 50 random samples of 500 data points, totalling the 25,000 observation data points. Each observation had 7 features: the Median filters with three different window sizes, Savistzky-Golay, Wavelet and two gradient features. These features were used to distinguish the transition observations from the steady observation relative to a time axis. Fig. 3 show a sample data for the decreasing trend.

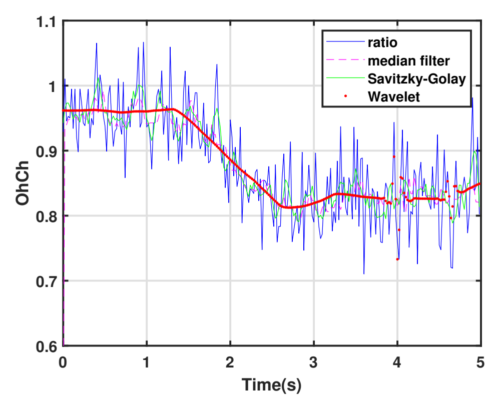

Figure 3: OHCH Ratio and Features

3 MACHINE LEARNING ALGORITHMS

For this research Support Vector Machines (SVMs) and Feedforward Neural Networks (FNNs) were chosen, although they are two alternative machine learning approaches for classification and regression problems with different inductive bias and very interesting properties. They however share a number of elements that allow use to be able to establish a direct correspondence between them. In fact, from a formal point of view, they are structurally similar [16].

3.1 Support Vector Machine (SVM)

A Support Vector Machine (SVM) as seen in Fig. 4, is a supervised machine learning technique derived from two foundations: Statistical Learning Theory and Mathematical Optimization, applied for classification, regression, and other learning tasks showing high performance in practical applications [2, 6, 9, 14]. It determines the limits of a decision, producing a great separation between classes by minimizing the errors. For this, SVM implements two basic mathematical operations: non-linear mapping of input vectors in a high dimensional feature space (kernels), and constructing a maximum margin hyperplane in the feature space. The construction of this hyperplane is performed in accordance with the principle of structural risk minimization (SRM). Using hyperplanes, SVM discovers the boundaries between the input classes and the input elements defining the boundaries and from the training data a maximum margin hyperplane splits the data so that the distance between the margin and the hyperplane is maximized. For more details on SVM see Refs [1, 3, 7, 20].

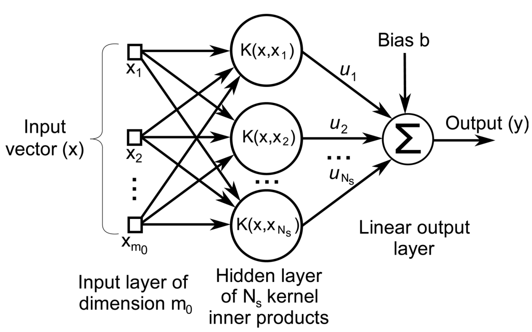

Figure 4: Architecture of a Support Vector Machine Classifier[17]

The SVM classifier is provided in the Classification Learner App in MATLAB. While MATLAB possesses a number of variations of the SVM, the Fine Gaussian model was chosen as it enables high model flexibility and is capable of making fine and accurate class distinctions [13]. This type of SVM also helped to define linear separability between multi-dimensional data where prior knowledge about the data isn't required [4]. The data was also automatically standardized by scaling the distance between the predictors so fitting would improve, thus avoiding overfitting or underfitting issues [13]. The model was trained using the default optimizer parameters provided by MATLAB.

3.2 Basic Feedforward Neural Network

Often referred to as a multi-layered network of neurons, the Feedforward Neural Networks (FNN) consists of a series of fully connected layers that connect every neuron in one layer to every neuron in the other layer (Fig. 5). It comprises 4 components - (i) the input layer that contains the neurons that receive inputs and pass them on to the other layers. The number of neurons in the input layer should be equal to the attributes or features in the dataset; (ii) the hidden layer that is concealed between the input and output layers and is used to perform alterations on the inputs; (iii) the output layer that is the predicted/expected feature and depends on the type of model been built; and (iv) the neuron weights that refer to the strength or amplitude of a connection between two neurons and are often initialized between 0 and 1. The data therefore enters the input layer, travels through the hidden layers, and eventually exits the output nodes. The network is devoid of links that would allow the information exiting the output node to be sent back into the network [18].

The major advantage of fully connected networks is that they are "structure agnostic" i.e. there are no special assumptions needed to be made about the input.

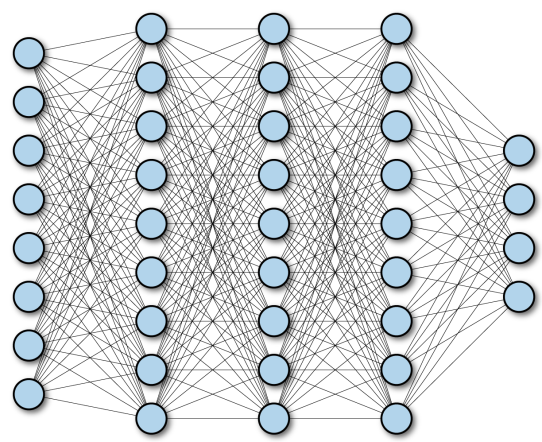

Figure 5: 3-layer Feed Forward Neural Network with a 8 Input Layers[15]

The FNN algorithm was also provided in MATLAB. It is a feedforward, fully connected neural network with 3 possible layers. The first layer has a connection from the input, and each subsequent layer weight matrix and then a bias vector is added. The ReLU activation function follows each fully connected layer. The final fully connected layer and the subsequent softmax activation function produce the output.

3.3 Approach

To conduct the research the datasets were first prepared through the processing of denoising through the use of different filters. The different steps involved in denoising the chosen dataset and comparing the filters can be summarized as shown below:

- Collection of signal or time-series data (if not already noisy, random noise may need to be generated)

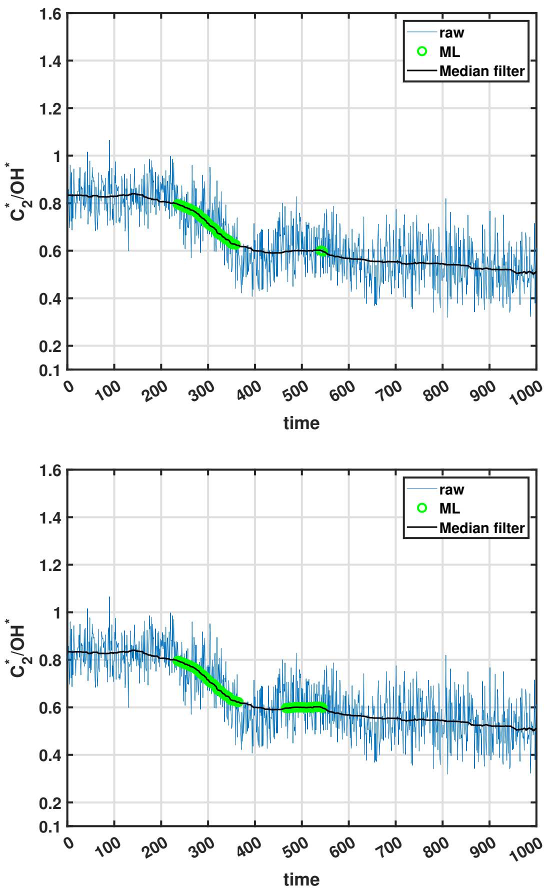

Figure 6: Detecting real UVA data using (a) SVM, (b) FNN for the decreasing transition

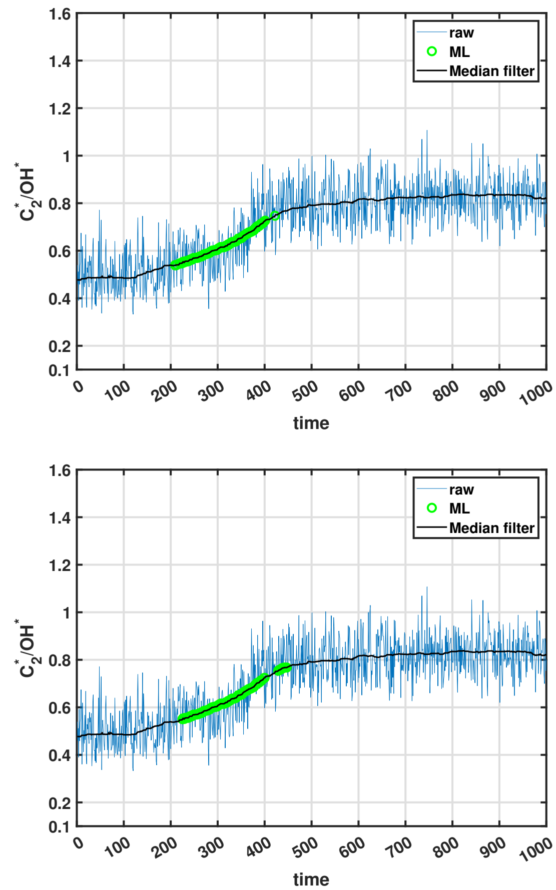

Figure 7: Detecting real UVA data using (a) SVM, (b) FNN for the increasing transition

- Utilization of MATLAB's denoising filter functions with empirical parameters to generate denoised datasets or feature sequences.

The training data (the seven feature sequences and a classification sequence) was then loaded in the two classification algorithms: SVM and FNN in MATLAB Classification Learner app with default settings. The FNN was tested using 1, 2 and 3 layers. For both algorithms the network's output, namely classification scores (posterior probabilities) and predicted labels were collected and compared.

4 RESULTS AND DISCUSSION

Analysis of each algorithm performance can be determined using a Confusion Matrix. From this we could determine how often each algorithm was correct (accuracy) and how often did they predict the answer as yes (True Positive Rate - TPR). For this research the results for the 4 tests can be seen in Table 1 which shows the TPR for the algorithms to detect the transition state of the OES signals and overall accuracy for both states. It can be seen that all 4 tests were comparable in their accuracy. Their TPR shows the main difference - 3-layer FNN has the best TPR, indicating that it provided the best detection of the transitions in the signals.

Table 1: Classifiers Results for DataSet (%)

Classifier	Predicted Class (TPR)	Overall Accuracy
SVM	93.0	97.8
1-Layer NN	92.8	97.9
2-Layers NN	93.0	97.8
3-Layers NN	93.1	97.8

Both SVM and FNN were used to detect transition states in both simulated (Fig. 8) and real datasets (Fig. 6 and Fig. 7). In both cases the raw data is represented as blue, the filtered result as black and the red dots denoting the true transition time points. In both datasets the algorithms were able to detect increasing and decreasing transitions.

For the simulated data where there were true transitions, in both algorithms there were little harmful false positives. Fig. 8 shows examples of transition results for both algorithms.

For the real dataset where there were no true transitions, both SVM and FNN were able to detect the transition states. It was found however that FNN had more false positives during the steady states

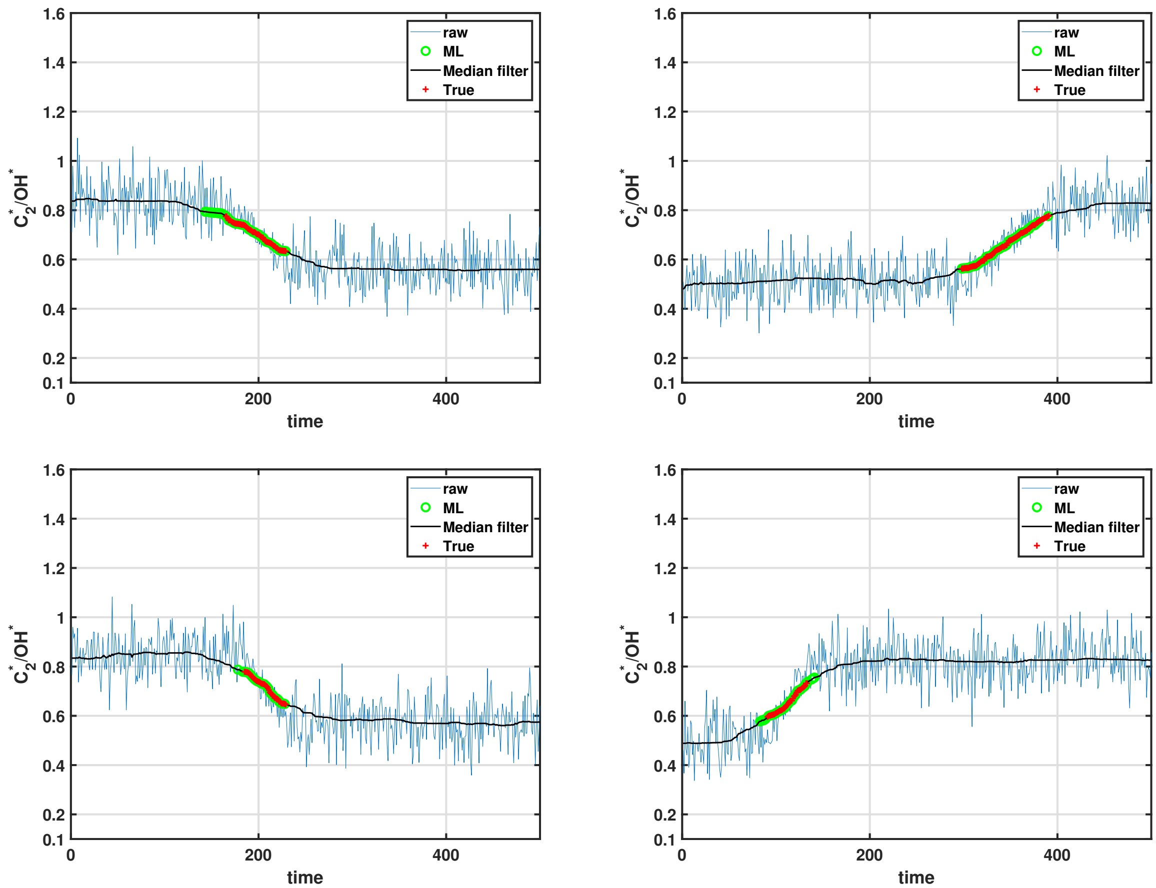

Figure 8: Detecting simulated data using (a)(b) SVM, (c)(d) FNN

than SVM. Fig 6 and Fig 7 show examples of transition results for both algorithms.

5 CONCLUSION

The goal of this research is to detect the transition that occurs in OES sensor data. In our experiments, FNNs obtained similar accuracies to SVMs when detecting these transitions with nearly 98% accuracy. This occurred no matter the filtering algorithm utilized. Experimentation showed however that FNN produce more true predictions that SVM.

The experimentation therefore generated questions that call for additional testing and future work. In reference to the SVM classification model, various methods can be taken for its improvement. Since FNN performed better with more layers there can be more tests with more layers. Another possibility is the testing with more algorithms including Deep Learning algorithms.

6 ACKNOWLEDGEMENTS

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