Machine Learning as an Online Diagnostic Tool for PEM Fuel Cells

Shangwei Zhou [a], Paul. R. Shearing [a], Dan J. L. Brett [a], Rhodri Jervis [a,*]

[a] *Electrochemical Innovation Lab, Department of Chemical Engineering, University College London, Torrington Place, WC1E 7JE, London, UK*

* *Corresponding author.*
E-mail address: rhodri.jervis@ucl.ac.uk

Abstract

Proton exchange membrane (PEM) fuel cells are considered a promising power supply system with high efficiency and zero emissions. They typically work within a relatively narrow range of temperature and humidity to achieve optimal performance; however, this makes the system difficult to control, leading to faults and accelerated degradation. Two main approaches can be used for diagnosis; limited data input which provides an unintrusive, rapid but limited analysis, or advanced characterisation that provides a more accurate diagnosis but often requires invasive or slow measurements. In order to provide an accurate diagnosis with rapid data acquisition, machine learning (ML) methods have shown great potential. However, there is a broad approach to the diagnostic algorithms and signals used in the field. This paper provides a critical view of the current approaches and suggests recommendations for future methodologies of ML in fuel cell diagnostic applications.

Keywords: Proton Exchange Membrane Fuel Cell (PEMFC); Fault diagnosis; Water management failure; Machine learning; Data-driven.

Introduction

Fuel cells are electrochemical energy generators, converting chemical energy into electricity and heat directly. They have attracted growing attention in automotive and stationary applications, thanks to their zero emissions, high energy conversion efficiency and power density. Two systems have attracted a lot of attention and development: proton exchange membrane (PEM) fuel cells and solid oxide fuel cells (SOFCs) [1], named for the type of electrolyte they use.

Cost is one of the significant barriers to commercialising PEM fuel cells [2], mainly due to the high Pt load on the cathode side and small batch production. Another important hinderance is insufficient durability and reliability [3]. Consequently, various fault diagnosis techniques and fault tolerance control strategies have been developed. The former can detect and identify faulty modes, and the latter adapts to correct developing faults and maintain optimal performance. Petrone et al. [4] proposed an overview of different model-based diagnosis approaches and Zheng et al. [5] have presented a complementary review on non-model diagnosis methodologies. Both works suggest that data-driven methods may be a promising solution for online fuel cell diagnosis. It is worth mentioning that Machine learning (ML) algorithms have also performed well in material and structure optimisation [6, 7], remaining lifetime prediction [8] and other fields of fuel cells.

PEM fuel cell fault modes

A typical fuel cell system is composed of the fuel cell stack (containing catalyst-coated electrodes and a polymer electrolyte membrane – together termed the membrane electrode assembly, MEA), reactant supply subsystems, humidification, coolant circuits, a DC/DC converter and a controller unit. The operating conditions of the system are complicated and can be affected by many external factors, meaning faults may occur in different components during the life-cycle, resulting in a temporary decrease in system performance or accelerated degradation of the MEA or balance-of-plant (BOP).

Faults can be divided into 'recoverable' and 'unrecoverable'. An unrecoverable fault generally refers to a permanent structural defect; for instance, pinholes or flaws in the membrane formed during the stack compression or assembly [9], or operational chemical degradation [10].

The 'recoverable' faults are those whereby the reduction in system performance is temporary and can be reversed with appropriate actions, such as short-circuit [11], reactant starvation, impurity poisoning (CO, H_2S, and NH_3) and water management failures [12]. However, if there is no timely fault detection and handling mechanism in the system, a reversible fault evolves into an irreversible one; for instance, Taniguchi et al. [13] analysed the effect of hydrogen starvation and showed that the cell output voltage rapidly drops below zero when the anode is short on fuel (termed cell reversal).

Water management failures are the most commonly encountered and represent over 50% of PEM fuel cell faults [14]. Especially for the next generation of self-humidifying fuel cell systems, water management will be critical to optimal performance. There is a subtle balance between the generation, transport and removal of water to maintain a stable voltage output [15, 16]. Once a fault occurs, it should be detected and identified as quickly as possible by a non-intrusive and real-time tool; it can then often be mitigated or even eliminated.

Intrusive diagnostic techniques

Intrusive diagnostic approaches give us a fundamental understanding of degradation mechanisms caused by various faults and they are generally *ex-situ* diagnostic tools or involve pausing the operation of the fuel cell to carry out *in situ* testing. Examples include electrochemical impedance spectroscopy (EIS) [17-20], cyclic voltammetry (CV) [21, 22], galvanostatic analysis [23, 24], and visualization [25-27] or spectroscopic measurements [28]. They can provide detailed information about the state-of-health (SoH) of the fuel cell system or materials; nevertheless, they typically require special modifications to the fuel cell system, which can affect its integrity (such as altered external components allowing probing of the MEA), or changing the nominal operating conditions. Additionally, since sensors cannot directly measure all faults, building the reverse relationship between system characteristics and SoH is challenging. Model-based approaches involve modelling the fuel cell system and then comparing the model outputs with the sensor measurements, the residual signal determining the SoH. This can be a complex and computationally demanding process; however, methods based on ML do not require a complex system model and fitting parameters.

Instead, they establish a mapping function between signal and SoH directly.

Traditional ML-based diagnostic techniques

ML refers to a process whereby an algorithm is used to obtain models from data or interaction with the environment that can then be run automatically with minimal human interaction. ML can be divided into unsupervised, supervised or reinforcement learning. From the perspective of the training process, unsupervised learning only uses unlabeled datasets, supervised learning uses labelled datasets, and reinforcement learning needs dynamic interaction with the environment. Reinforcement learning addresses the decision-making problem of maximising long-term rewards. For example, Zhou et al. [29] proposed reinforcement learning-based energy management strategies for fuel cell vehicles to achieve maximum service lifetime of two power sources. Unsupervised learning is concerned with the distribution of the data itself. One of the common methods is clustering, which can group data points with similar characteristics or features. When the label takes the continuous value in supervised learning, it is called a regression problem, and when the label bears the discrete value, it is a classification problem. Therefore, data-driven fault diagnosis can be considered a classification problem.

Figure 1 shows a simplified workflow of how ML can be used in fuel cell fault diagnosis. In the data collection step, experiments need to be carried out at different operating conditions, including fault free and other faulty states of interest, and the method of faults being imposed requires careful design. Then, the ML-based diagnostic model is trained, and so the relationship between the signal and SoH is built. Finally, the model can be deployed in a fuel cell system to monitor SoH online. The two most critical factors are the signals and the diagnostic model, as shown in Fig. 1. The diagnostic signals should be as simple as possible under the premise of indicating faults. Signals reflecting SoH include individual cell voltages [30-32], magnetic fields [33, 34], current density distribution [35, 36], acoustic emission [37, 38] and impedance spectra [39].

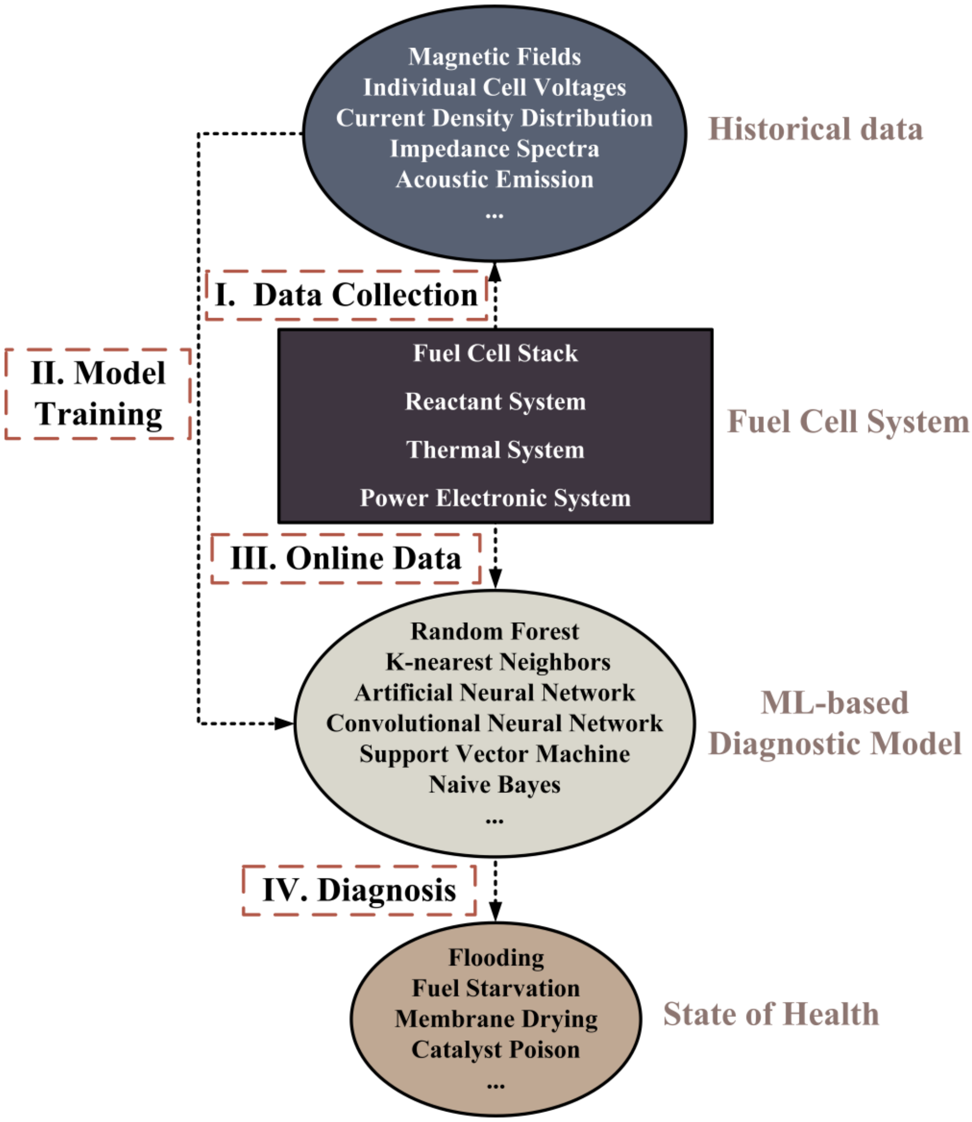

Fig. 1. Flowchart of the ML-based diagnostic techniques as applied to a fuel cell system.

Li et al. [31] used Fisher discriminant analysis (FDA) to extract low dimensional features from the individual cell voltages. FDA makes it possible to separate data from different classes after dimensionality reduction. A PEMFC stack is typically composed of dozens or hundreds of cells, so feature extraction is necessary before training the classifier. The spherical-shaped multiple-class support vector machine (SSM-SVM) is adopted to classify the features into different SoH. Compared to the original SVM, SSM-SVM overcomes the limitation of being unable to recognise an unknown class – that is if the model is trained with only two classes (say ‘humidified’ and ‘dry’). For a class outside of the training dataset (such as ‘catalyst poisoning’), SVM will also recognise it as humidified or dry. Therefore, even if the new sample belongs to an unknown fault, conventional classifiers falsely predict it to be one of the predefined faults, but the SSM-SVM will classify it as a potential novel SoH. Li et al. [32] further verified the effectiveness of FDA by combining a directed acyclic graph SVM classifier as the diagnostic structure with experimental data from two different sized stacks, and other works provide online validation [40, 41]. As shown in Fig. 2a, the diagnostic methods based on ML include two procedures: offline and online, where offline training includes diagnostic model training and verification. Mao et al. [42] used stack voltage, current and operating conditions as the original diagnostic signals. The performance of supervised kernel FDA and unsupervised kernel principal component analysis (PCA) as the feature extraction algorithm is also compared. Unlike FDA, PCA aims to maximize the variance of the original data in the feature space. The introduction of the kernel function maps the original samples to higher dimensional space, which is used to solve the case of linear inseparability. Liu et al. [43] presented a diagnostic strategy based on the K-means clustering algorithm and discrete hidden Markov model (DHMM). K-means is an unsupervised iterative clustering algorithm whereby K clustering centers are randomly selected, and each data point is assigned to the nearest clustering center. Then, the average vector of each class is used as the clustering center of the next iteration. The singular sample points can be screened out in the data processing stage, and the K-value is set to the number of health states (6 here), then the original data of the same health state will be grouped. The point where the health state contradicts the grouping is singular. The average diagnostic accuracy for six different health states is 94.17% achieving higher classification accuracy than SVM with less computational cost. To deal with simultaneous faults in SOFCs, multi-label SVM was employed by Li et al. [44], which only requires a training dataset of a single isolated fault. Although there are many differences between SOFCs and PEMFCs, the fault diagnosis strategy and the challenges are referential. Lin et al. [45] applied incremental PCA as the feature extraction algorithm, and four different classifiers are compared, concluding that random forest classifiers worked best. Liu et al. [46] presented a conversion technique to transform time-series cell voltage signals into 2D images, the statistical features of which are then extracted and classified by K-means.

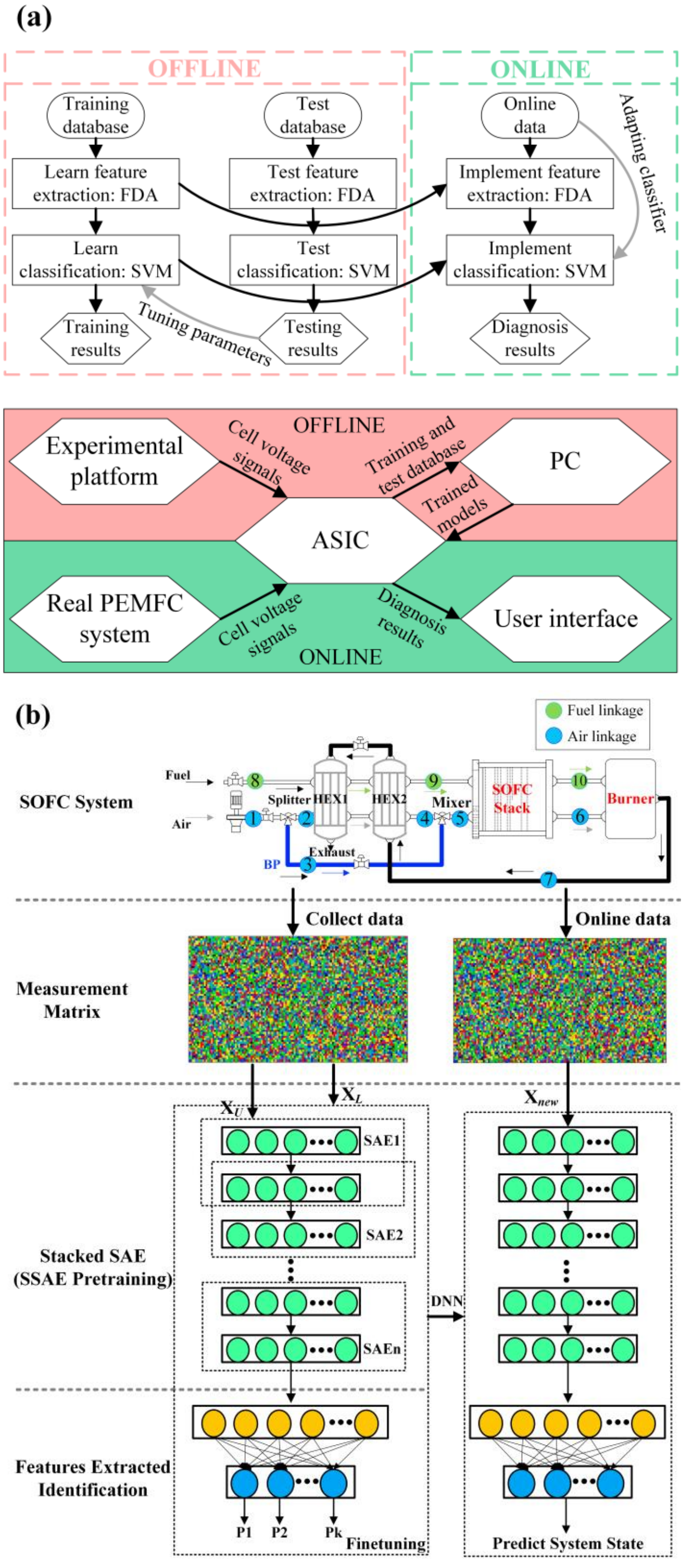

Fig. 2. The implementation procedure of the ML-based diagnostic strategies. Figure (a) adapted and rearranged with permission from Li et al. [41], Copyright (2018) Elsevier. Figure (b) adapted and rearranged with permission from Zhang et al. [47], Copyright (2018) Elsevier.

Neural networks have also shown the strong capability, including reservoir computing [48, 49], extreme learning machine (ELM) [50], stacked sparse autoencoder

(SSAE) [47] and long short-term memory (LSTM) networks [51, 52]. Liu et al. [50] combined ELM and Dempster–Shafer (D-S) theory to study the diagnostic result fusion at the decision level. The average recognition rate reaches 98.70%, and the operating time is only 0.211 s. ELM is a fast algorithm to solve the weight and bias of the single hidden layer neural network without calculating the gradient of the loss function. Since many signals are correlated with the SoH, the fusion problem arises correspondingly, and the fusion is divided into data fusion and decision fusion. Data fusion refers to splicing signals from different sensors, followed by input into the unique diagnostic model. Decision fusion here refers to determining the final result when multiple diagnostic models have different predictions. D-S theory is a framework for reasoning with uncertainty. Zhang et al. [47] proposed an SSAE-based diagnostic strategy for simultaneous faults (Fig. 2b). The diagnostic model parameters can be pre-trained with large amounts of unlabeled samples, and then fine-tuned with small amounts of labelled samples. Gu et al. [52] integrated the LSTM model into the embedded system (Simulink/C) and realised the online diagnosis (system controller) of flooding faults. LSTM can effectively process time-series signals, the traditional neural network does not consider the relationship between the current and previous output, so it cannot handle sequence data well. LSTM has the ability to handle long-term dependency problems thanks to its gates structure, meaning that LSTM networks can provide more reasonable diagnositic results compared to other "memoryless" approaches.

ML-based techniques do not require physical parameters and theoretical relationships of the system. The SoH of the fuel cell system can be recognised through identifying patterns from simple sensor signals; therefore, they can be a suitable solution for real-time application in SoH determination.

From the laboratory concept to the industrial application of ML-based methods, the primary consideration remains: how to achieve high diagnostic accuracy through low-cost sensors, followed by the reliability and robustness of the diagnostic model. The sensor fault is considered by Zhao et al. [53] and Mao et al. [54].

Deep learning era

Fuel cell systems usually work at dynamic load under different operating conditions. Lim et al. [55] achieved >92% diagnostic accuracy under untrained current densities using the residual basis scaling method, but the reliability is insufficient. Traditional ML algorithms have been applied to most fault diagnosis cases, but they only perform well on signals with the same distribution as their training data. Convolutional neural networks (CNNs) and the following signal-to-image conversion technique have the potential to solve this problem, an example as illustrated in Fig. 3b. The single cell voltages can be transformed into images, and then CNN is used instead of traditional ML models. In the field of target detection, before the deep-learning era, feature vector extraction and following classification are the typical steps; this is the same as data-driven fault diagnosis of fuel cells. However, object detection achieved remarkable progress based on deep-learning techniques, such as R-CNN [56], Faster R-CNN [57], YOLO [58], SSD [59], thanks to their ability to generalise untrained samples. Besides, CNN is an end-to-end diagnostic model, which does not require the feature extraction/selection step (Fig. 3a).

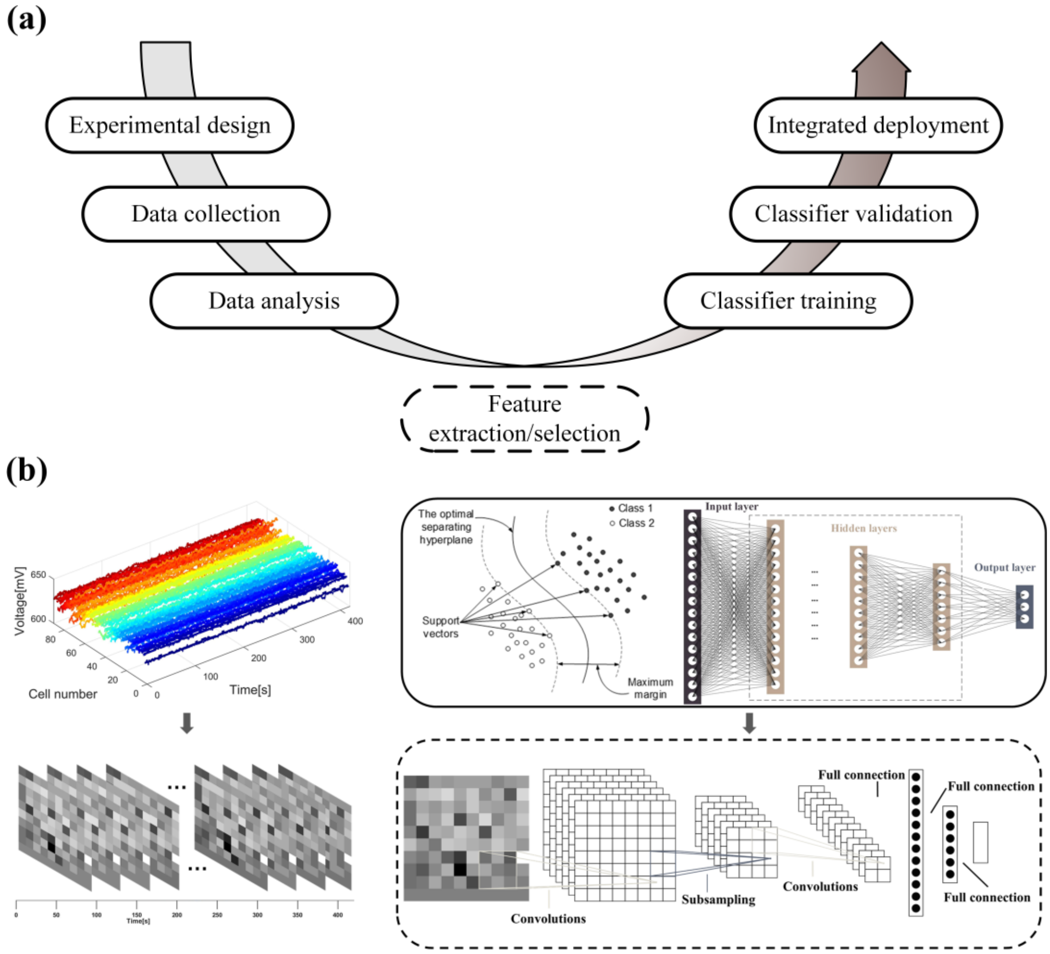

Fig. 3. Fault diagnosis evolving from traditional ML to deep learning using signal-to-image conversion techniques. The individual cell voltages figure reproduced and adapted with permission from Zhou et al. [30], Copyright (2020) Elsevier.

ML-based fault diagnosis is still in the stage of model verification, using test data to verify the diagnosis model's effectiveness. The possible challenges of integrating to the onboard controller, such as limited computation ability and time delay, have not yet been considered. Fault diagnosis aims to improve the recognition rate to 100% if possible. However, a single diagnostic model can only obtain a limited recognition capability which may be insufficient for the actual application [60]. Decision fusion systems have received significant attention, and the cooperation of different classifiers ultimately performs better than the outcome of a single one, just like the double-negative test for Coivd-19 (a PCR swab and an IgM antibody test). It allows for avoidance of the uncertainties of the individual diagnostic approach. The performance of four decision fusion techniques, including majority voting, Bayesian belief, multi-agent and modified Borda count, are explored by Niu et al. [61]. The accuracy of Bayesian belief could reach 100%, which is a remarkable improvement compared with the 74% accuracy rate of the best individual classifier.

Data-driven fault diagnosis approaches are in the early stages of laboratory testing, with training sample data for each SoH in the literature ranging from dozens to thousands of data sets. In general, the reliable size of the training dataset depends on the requirements for the diagnostic model. If the diagnostic model requires different loads, the training dataset also needs to include a wide range of load conditions. Even under the same load, the severity of faults varies due to the fluctuation of operating conditions. The larger the training data is, the more information it contains and the more accurate the ML prediction will be. Open source training and test datasets will facilitate the optimisation of diagnostic methods for researchers unable to perform costly fault embedding experiments.

Conclusions

The realisation of real-time fault diagnosis can evaluate the control strategy of fuel cell systems. It can even correct the operating condition by integrating into the control logic, avoiding recoverable fault deterioration, and improving the fuel cell system's reliability and durability. Effort in improving diagnostic accuracy and reducing computational costs is needed, and other problems such as the generalisation ability, decision fusion and online deployment of the diagnostic model also remain.

Cross-fertilisation of strategies adopted for lithium-ion battery systems would be helpful [62-64]. Finally, micro-integrated sensors can provide more sensitive and robust signals for ML-based fault diagnosis techniques, improving the accuracy of such models and ultimately leading to rapid onboard fault detection and prevention methodologies.

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