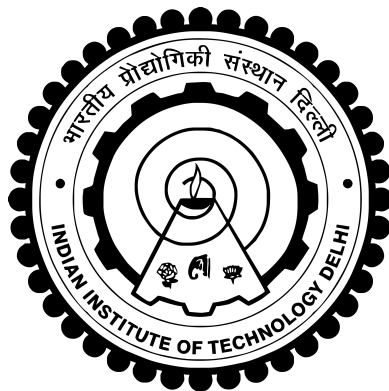


DATA-DRIVEN PROCESS FAULT DETECTION
USING MACHINE LEARNING TECHNIQUES

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DEPARTMENT OF CHEMICAL ENGINEERING
INDIAN INSTITUTE OF TECHNOLOGY DELHI

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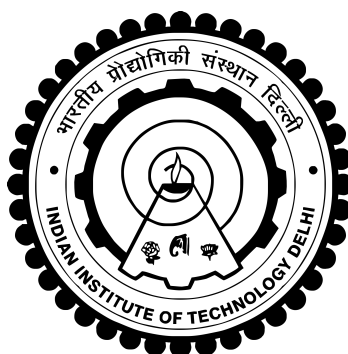
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THESIS CERTIFICATE

This is to certify that the thesis titled **Data-driven Process Fault Detection using Machine Learning and Deep Learning Techniques**, submitted by **Jyoti Rani (2019CHZ8165)**, to the Indian Institute of Technology, Delhi, for the award of the degree of **Doctor of Philosophy**, is a bonafide record of the research work done by her under our supervision. The contents of this thesis, in full or in parts, have not been submitted to any other Institute or University for the award of any degree or diploma.

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Jyoti Rani

ABSTRACT

In response to the escalating volume and intricacy of data in critical domains such as cybersecurity, finance, healthcare, and industrial processes, the need for robust anomaly detection methods has become increasingly pressing. This thesis undertakes a comprehensive exploration into the effectiveness of machine learning and deep learning techniques for detecting anomalies within large-scale datasets. The investigation encompasses both supervised and unsupervised learning algorithms, coupled with cutting-edge deep learning architectures, to address the complex challenges associated with anomaly detection in dynamic environments. Commencing with a thorough review of existing literature on anomaly detection methods, the research identifies gaps and emphasizes the importance of data-driven approaches for achieving heightened accuracy and adaptability. The thesis introduces novel methodologies that intricately integrate machine learning algorithms with deep learning techniques, aiming to synergize their unique strengths and elevate detection capabilities across diverse anomaly patterns. Subsequent chapters delve into detailed case studies and real-world applications of these methodologies.

Chapter 3 of the thesis focuses on the safety and reliability of pressurized heavy water nuclear reactors (PHWRs), employing a staged procedure for fault detection using Gaussian Mixture Models (GMM), Hidden Markov Model (HMM), and Probabilistic Principal Component Analysis (PPCA). PHWR operation involves various operational modes and dynamic transitions, posing challenges for fault detection. Various frameworks, such as clustering parameters and iterative Principal Component Analysis (PCA), have been explored in the literature. Inspired by these, the study presents a data-driven fault detection case study of a Canada Deuterium Uranium (CANDU) type large Indian PHWR using simulated data and real-time operational plant data. A staged procedure, including mode identification and clustering of Normal Operating Condition (NOC) data through the Hidden Markov Model (HMM), is employed. The proposed approach integrates the HMM and Probabilistic Principal Component Analysis (PPCA) for steady mode identification and Dynamic Principal Component Analysis (DPCA) for modeling dynamic operation. The performance is

evaluated using monitoring charts, and statistical parameters, and benchmarked against conventional methods.

In subsequent chapter 4 of the thesis recognizing the challenge of obtaining accurately labeled data for anomaly detection, an unsupervised method using Generative Adversarial Auto-Encoders (GAAE) is introduced. The GAAE, utilizing Wasserstein loss with gradient penalty and cycle consistency loss, is proposed. GANs, being unsupervised models, can learn the underlying structure of normal time series data without the need for labeled anomalies, making them suitable for scenarios where anomalous patterns are diverse and challenging to define. GANs can also capture the multimodal nature of anomalies by generating various plausible instances of abnormal patterns. This can be beneficial for detecting anomalies with different characteristics. The Autoencoder framework effectively captures hidden data distributions, and the Wasserstein loss with gradient penalty addresses issues such as mode collapse. The cycle consistency loss further ensures the consistency of generated data. The proposed method is evaluated for fault detection using Tennessee Eastman benchmark data and real-time industrial-scale nuclear power flux data, demonstrating promising results in various deep learning-based modeling tasks.

In Chapter 5 of the thesis delves into fault detection and isolation within dynamic processes. The focal point is the introduction of the Probabilistic Wavelet Neural Operator Auto-Encoder (PWNOAE), an extended version of the Wavelet Neural Operator (WNO) infused with a probabilistic framework. The PWNOAE seamlessly integrates wavelet analysis, neural operators, and probability theory to capture the distribution of infinite-dimensional multivariate input. This approach is chosen for its aptitude in incorporating prior knowledge or known physical principles into the learning process, particularly beneficial in anomaly detection scenarios where domain-specific insights can enhance the model's understanding of normal behavior. The suitability of neural operators in handling infinite-dimensional input is emphasized, a critical aspect in the context of anomaly detection. Time series data often exhibits infinite-dimensional characteristics, especially when considering temporal dependencies and variations.

The PWNOAE, by design, leverages this characteristic to effectively model complex relationships inherent in dynamic processes. The probabilistic extension of the Wavelet Neural Operator in the PWNOAE brings additional advantages. This includes the ability to capture uncertainty and variability in the data distribution, a pivotal feature when dealing

with anomalies characterized by uncertain patterns. By training the PWNOAE on healthy field measurements and testing on real-time measurements, the model is equipped for fault detection. The online predictions' uncertainty becomes a valuable indicator of anomalies, enabling the isolation of faults by scrutinizing prediction uncertainty in individual variables. To substantiate the efficacy of the proposed method, benchmark data and industrial data from a pressurized heavy-water nuclear reactor are employed. The results showcase the notable success of the PWNOAE in detecting and isolating faults, demonstrating superior performance when compared to established baselines.

Recognizing the limitations of existing models in accurately capturing multivariate probability distributions, Chapter 6 of the thesis introduces a novel approach: the Generative Adversarial Wavelet Neural Operator (GAWNO). This innovative approach intertwines classical GAN principles with a U-Net architecture for generator and discriminator modules, resulting in heightened accuracy in comprehending intricate multivariate distributions. Within this framework, GANs, complemented by neural operators, establish a system where the generator endeavors to replicate real data, while the discriminator works to distinguish between authentic and generated data. Within this context, neural operators, acting as embedded mathematical operations in the GAN architecture, augment the model's capacity to apprehend intricate functions and relationships within time series data. GAWNO harnesses neural operators to seize and model the inherent dynamics of time series data, merging the generative capabilities of GANs with the frequency analysis facilitated by wavelet transforms. Validation of this pioneering methodology is carried out using datasets sourced from the Tennessee Eastman Process simulation and Avedore wastewater treatment plant, demonstrating promising results that outshine established benchmarks in the literature.

In conclusion, this thesis makes various contributions by presenting novel methodologies, frameworks, and practical insights that showcase promising results in diverse industrial settings. Bridging the gap between traditional machine learning and cutting-edge deep learning and the new area of operator learning research offers a comprehensive guide for practitioners and researchers seeking effective anomaly detection solutions. The outcomes hold considerable potential to impact industries reliant on anomaly detection for safety, quality control, fraud detection, and system monitoring, fostering a more secure, efficient, and resilient data-driven environment.

KEYWORDS: Process monitoring; Fault detection and isolation; Probability distribution;

Autoencoders; Neural Operator; Wavelets; Hidden Markov models; Generative adversarial network

सारांश

साइबर सुरक्षा, वित्त, स्वास्थ्य सेवा और औद्योगिक प्रक्रियाओं जैसे महत्वपूर्ण क्षेत्रों में डेटा की बढ़ती मात्रा और जटिलता के जवाब में, मजबूत विसंगति का पता लगाने के तरीकों की आवश्यकता तेजी से बढ़ रही है। यह थीसिस बड़े पैमाने पर डेटासेट के भीतर विसंगतियों का पता लगाने के लिए मशीन लर्निंग और डीप लर्निंग तकनीकों की प्रभावशीलता में एक व्यापक अन्वेषण करता है। जांच में गतिशील वातावरण में विसंगति का पता लगाने से जुड़ी जटिल चुनौतियों का समाधान करने के लिए अत्याधुनिक गहन शिक्षण संरचनाओं के साथ पर्यवेक्षित और अनसुपरवाइज़्ड लर्निंग एल्गोरिदम दोनों शामिल हैं। विसंगति का पता लगाने के तरीकों पर मौजूदा साहित्य की गहन समीक्षा के साथ शुरू करते हुए, शोध अंतराल की पहचान करता है और उच्च सटीकता और अनुकूलनशीलता प्राप्त करने के लिए डेटा-संचालित दृष्टिकोण के महत्व पर जोर देता है। थीसिस नई पद्धतियों का परिचय देती है जो मशीन लर्निंग एल्गोरिदम को गहरी सीखने की तकनीकों के साथ जटिल रूप से एकीकृत करती है, जिसका उद्देश्य उनकी अनूठी शक्तियों को समन्वित करना और विविध विसंगतियों के पैटर्न में पहचान क्षमताओं को बढ़ाना है। बाद के अध्यायों में इन पद्धतियों के विस्तृत केस स्टडी और वास्तविक दुनिया के अनुप्रयोगों पर प्रकाश डाला गया है।

थीसिस का अध्याय 3 दबाव वाले भारी जल परमाणु रिएक्टरों (पीएचडब्ल्यूआर) की सुरक्षा और विश्वसनीयता पर केंद्रित है, जो गॉसियन मिक्सचर मॉडल (जीएमएम) हिडन मार्कोव मॉडल (एचएमएम) और प्रोबेबिलिस्टिक प्रिंसिपल कंपोनेंट एनालिसिस का उपयोग करके फॉल्ट डिटेक्शन के लिए एक चरणबद्ध प्रक्रिया को नियोजित करता है। (PPCA). पीएचडब्ल्यूआर संचालन में विभिन्न परिचालन मोड और गतिशील संक्रमण शामिल हैं, जो दोष का पता लगाने के लिए चुनौतियां पेश करते हैं। साहित्य में क्लस्टरिंग पैरामीटर और पुनरावृत्ति प्रधान घटक विश्लेषण (पी. सी. ए.) जैसे विभिन्न ढांचे का पता लगाया गया है। इनसे प्रेरित होकर, यह अध्ययन कनाडा ड्यूटेरियम यूरेनियम (सी. ए. एन. डी. यू.) प्रकार के बड़े भारतीय पी. एच. डब्ल्यू. आर. का डेटा-संचालित फॉल्ट डिटेक्शन केस स्टडी प्रस्तुत करता है, जिसमें सिम्युलेटेड डेटा और रियल-टाइम ऑपरेशनल प्लांट डेटा का उपयोग किया जाता है। हिडन मार्कोव मॉडल (एच. एम. एम.) के माध्यम से सामान्य परिचालन स्थिति (एन. ओ. सी.) डेटा की मोड पहचान और क्लस्टरिंग सहित एक चरणबद्ध प्रक्रिया नियोजित है। प्रस्तावित दृष्टिकोण गतिशील संचालन मॉडलिंग के लिए स्थिर मोड पहचान और गतिशील प्रधान घटक विश्लेषण (डी. पी. सी. ए.) के लिए एच. एम. एम. और संभावित प्रधान घटक विश्लेषण (पी. पी. सी. ए.) को एकीकृत करता है। प्रदर्शन है निगरानी चार्ट और सांख्यिकीय मापदंडों का उपयोग करके मूल्यांकन किया जाता है और पारंपरिक तरीकों के खिलाफ बेंचमार्क किया जाता है।

थीसिस के बाद के अध्याय 4 में विसंगति का पता लगाने के लिए सटीक रूप से लेबल किए गए डेटा प्राप्त करने की चुनौती को पहचानते हुए, जनरेटिव एडवर्सियल ऑटो-एन्कोडर्स (जी. ए. ए. ई.) का उपयोग करते हुए एक अनसुपरवाइज़्ड विधि पेश की गई है। जी. ए. ए. ई., ढाल दंड और चक्र स्थिरता हानि के साथ वासरस्टीन हानि का उपयोग करते हुए, प्रस्तावित है। जी. ए. एन., अनसुपरवाइज़्ड मॉडल होने के नाते, लेबल विसंगतियों की आवश्यकता के बिना सामान्य समय श्रृंखला डेटा की अंतर्निहित संरचना को सीख सकते हैं, जिससे वे उन परिदृश्यों के लिए उपयुक्त हो जाते हैं जहां विसंगत पैटर्न विविध और परिभाषित करने के लिए चुनौतीपूर्ण होते हैं। जी. ए. एन. असामान्य पैटर्न के विभिन्न प्रशंसनीय उदाहरण उत्पन्न करके विसंगतियों की बहुआयामी प्रकृति को भी पकड़ सकते हैं। यह विभिन्न विशेषताओं वाली विसंगतियों का पता लगाने के लिए फायदेमंद हो सकता है। ऑटोएनकोडर फ्रेमवर्क

प्रभावी रूप से छिपे हुए डेटा वितरण को पकड़ता है, और ग्रेडिएंट पेनल्टी के साथ वासरस्टीन नुकसान मोड पतन जैसे मुद्दों को संबोधित करता है। चक्र स्थिरता हानि आगे उत्पन्न डेटा की स्थिरता सुनिश्चित करती है। प्रस्तावित विधि का मूल्यांकन टेनेसी ईस्टमैन बेंचमार्क डेटा और वास्तविक समय औद्योगिक पैमाने पर परमाणु ऊर्जा प्रवाह डेटा का उपयोग करके दोष का पता लगाने के लिए किया जाता है, जो विभिन्न गहन शिक्षण-आधारित मॉडलिंग कार्यों में आशाजनक परिणामों का प्रदर्शन करता है।

थीसिस के अध्याय 5 में गतिशील प्रक्रियाओं के भीतर दोष का पता लगाने और अलगाव पर प्रकाश डाला गया है। केंद्र बिंदु प्रोबेबिलिस्टिक वेवलेट न्यूरल ऑपरेटर ऑटो-एन्कोडर (पीडब्लूएनओई) की शुरुआत है, जो एक प्रोबेबिलिस्टिक फ्रेमवर्क के साथ वेवलेट न्यूरल ऑपरेटर (डब्ल्यूएनओ) का एक विस्तारित संस्करण है। पी. डब्ल्यू. एन. ओ. ए. ई. असीम-आयामी बहुभिन्नरूपी इनपुट के वितरण को पकड़ने के लिए वेवलेट विश्लेषण, तंत्रिका प्रचालक और संभाव्यता सिद्धांत को निर्बाध रूप से एकीकृत करता है। इस दृष्टिकोण को सीखने की प्रक्रिया में पूर्व ज्ञान या ज्ञात भौतिक सिद्धांतों को शामिल करने में इसकी योग्यता के लिए चुना जाता है, विशेष रूप से विसंगति का पता लगाने वाले परिदृश्यों में फायदेमंद है जहां डोमेन-विशिष्ट अंतर्दृष्टि सामान्य व्यवहार की मॉडल की समझ को बढ़ा सकती है। अनंत-आयामी इनपुट को संभालने में तंत्रिका प्रचालक की उपयुक्तता पर जोर दिया जाता है, जो विसंगति का पता लगाने के संदर्भ में एक महत्वपूर्ण पहलू है। समय श्रृंखला डेटा अक्सर अनंत-आयामी विशेषताओं को प्रदर्शित करता है, विशेष रूप से जब अस्थायी निर्भरताओं और भिन्नताओं पर विचार किया जाता है। पी. डब्ल्यू. एन. ओ. ए. ई., डिजाइन द्वारा, गतिशील प्रक्रियाओं में निहित जटिल संबंधों को प्रभावी ढंग से मॉडल करने के लिए इस विशेषता का लाभ उठाता है। पीडब्लूएनओई में वेवलेट न्यूरल ऑपरेटर का संभावित विस्तार अतिरिक्त लाभ लाता है। इसमें डेटा वितरण में अनिश्चितता और परिवर्तनशीलता को पकड़ने की क्षमता शामिल है, जो अनिश्चित पैटर्न द्वारा विशेषता वाली विसंगतियों से निपटने के लिए एक महत्वपूर्ण विशेषता है। स्वस्थ क्षेत्र मापन पर पीडब्लूएनओई को प्रशिक्षित करके और वास्तविक समय मापन पर परीक्षण करके, मॉडल दोष का पता लगाने के लिए सुसज्जित है। ऑनलाइन भविष्यवाणियों की अनिश्चितता विसंगतियों का एक मूल्यवान संकेतक बन जाती है, जो व्यक्तिगत चर में भविष्यवाणी अनिश्चितता की जांच करके दोषों को अलग करने में सक्षम बनाती है। प्रस्तावित विधि की प्रभावकारिता की पुष्टि करने के लिए, दबाव वाले भारी-जल परमाणु रिएक्टर से बेंचमार्क डेटा और औद्योगिक डेटा का उपयोग किया जाता है। परिणाम स्थापित आधार रेखाओं की तुलना में बेहतर प्रदर्शन का प्रदर्शन करते हुए दोषों का पता लगाने और उन्हें अलग करने में पीडब्लूएनओई की उल्लेखनीय सफलता को प्रदर्शित करते हैं।

बहुभिन्नरूपी संभाव्यता वितरणों को सटीक रूप से पकड़ने में मौजूदा मॉडलों की सीमाओं को पहचानते हुए, थीसिस का अध्याय 6 एक नए दृष्टिकोण का परिचय देता है: जेनेरेटिव एडवर्सियल वेवलेट न्यूरल ऑपरेटर (GAWNO). यह अभिनव दृष्टिकोण जनरेटर और डिस्क्रिमिनेटर मॉड्यूल के लिए यू-नेट वास्तुकला के साथ शास्त्रीय जीएन सिद्धांतों को जोड़ता है, जिसके परिणामस्वरूप जटिल बहुभिन्नरूपी वितरणों को समझने में सटीकता बढ़ जाती है। इस ढांचे के भीतर, जी. ए. एन., तंत्रिका प्रचालक द्वारा पूरक, एक ऐसी प्रणाली स्थापित करते हैं जहाँ जनरेटर वास्तविक डेटा को दोहराने का प्रयास करता है, जबकि विभेदक प्रामाणिक और उत्पन्न डेटा के बीच अंतर करने का काम करता है।

इस संदर्भ में, तंत्रिका प्रचालक, जी. ए. एन. वास्तुकला में अंतर्निहित गणितीय संचालन के रूप में कार्य

करते हुए, समय श्रृंखला डेटा के भीतर जटिल कार्यों और संबंधों को समझने के लिए मॉडल की क्षमता को बढ़ाते हैं। GAWNO न्यूरल ऑपरेटर्स का उपयोग समय श्रृंखला डेटा की अंतर्निहित गतिशीलता को पकड़ने और मॉडल करने के लिए करता है, GAN की उत्पादक क्षमताओं को वेवलेट ट्रांसफॉर्म द्वारा सुगम आवृत्ति विश्लेषण के साथ विलय करता है। इस अग्रणी पद्धति का सत्यापन टेनेसी ईस्टमैन प्रोसेस सिमुलेशन और अवेडोर अपशिष्ट जल उपचार संयंत्र से प्राप्त डेटासेट का उपयोग करके किया जाता है, जो आशाजनक परिणामों का प्रदर्शन करता है जो साहित्य में स्थापित मानकों को पीछे छोड़ देते हैं। अंत में, यह शोध प्रबंध नवीन पद्धतियों, रूपरेखाओं और व्यावहारिक अंतर्दृष्टि को प्रस्तुत करके विभिन्न योगदान देता है जो विविध औद्योगिक सेटिंग्स में आशाजनक परिणामों को प्रदर्शित करते हैं। पारंपरिक मशीन लर्निंग और अत्याधुनिक गहन शिक्षण और प्रचालक शिक्षण अनुसंधान के नए क्षेत्र के बीच की खाई को पाटना प्रभावी विसंगति का पता लगाने वाले समाधानों की तलाश करने वाले चिकित्सकों और शोधकर्ताओं के लिए एक व्यापक मार्गदर्शन प्रदान करता है। इन परिणामों में सुरक्षा, गुणवत्ता नियंत्रण, धोखाधड़ी का पता लगाने और प्रणाली की निगरानी, अधिक सुरक्षित, कुशल और लचीला डेटा-संचालित वातावरण को बढ़ावा देने के लिए विसंगति का पता लगाने पर निर्भर उद्योगों को प्रभावित करने की काफी क्षमता है।

कीवर्ड्स: प्रक्रिया की निगरानी; दोष का पता लगाना और अलगाव; संभाव्यता वितरण; ऑटोएन्कोडर; न्यूरल ऑपरेटर; वेवलेट; हिडन मार्कोव मॉडल; जनरेटिव प्रतिकूल नेटवर्क

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ABBREVIATIONS

IITD	Indian Institute of Technology, Delhi
DNN	Deep Neural Network
FD	Fault Detection
ZCC	Zonal Control Compartment
AE	Average Effectiveness
KDE	Kernel Density Estimation
FP	False Positives
MAR	Missed Alarm Rate
PCs	Principal Components
SPE	Squared Prediction Error
LZC	Liquid Zonal Control
NPP	Nuclear Power Plants
PPCA	Probabilistic Principal Component Analysis
PCA	Principal Component Analysis
DPCA	Dynamic Principal Component Analysis
SPM	Statistical process monitoring
PHWR	Pressurized Heavy Water Reactor
CANDU	Canada Deuterium Uranium
SVD	Singular value decomposition
NOC	Normal Operating Condition
NPCIL	Nuclear Power Corporation India Limited
NOC	Normal Operating Condition
GMM	Gaussian Mixture Models
NPP	Nuclear Power Plants
ARMA	Autoregressive Moving Average
ARIMA	AutoRegressive Integrated Moving Average
FDA	Functional Data Analysis

KPCA	Kernel Principal Component Analysis
KPLS	Kernel Partial Least Squares
KCVA	Kernel Canonical Variate Analysis
VAE	Variational autoen- coder
CAE	Convolutional autoencoders
LSTM-AE	long short-term memory autoencoders
GAN	Generative Adversarial Networks
WGAN	Wasserstein Generative Adversarial Networks
WIB	Wavelet integral blocks
BCE	Binary Cross Entropy
BiGAN	Bidirectional Generative Adversarial Network
FFT	Fast Fourier transform
FNO	Fourier Neural Operator
FNN	Forward Neural Network
DWT	Discrete Wavelet Transform
IDWT	Inverse Discrete Wavelet Transform
WNO	Wavelet Neural Operator
PWNOAE	Probabilistic Wavelet Neural Operator Auto-encoder
VAE	Variational autoen- coder
GWNO	Generative Wavelet Neural Operator

NOTATION

W	Weight matrix
λ	Decay constant of delayed neutron precursors
σ^2	Isotropic noise variance
ρ	Zonal reactivity
B_{th}	Threshold ratio
ϵ	Noise
Z	Latent variable
I	Identity matrix
S	Hidden states
\mathcal{A}	Input function spaces
\mathcal{U}	Output function spaces
Σ	Standard deviation
$\sigma(\cdot)$	Non-linear activation Function
\mathbf{l}	Linear transformation
$*$	Convolution operator
θ	Network parameter
\mathcal{W}	Wavelet transform
Ψ	Mother wavelet
τ	Scaling parameters
ζ	Shifting parameters
c_Ψ	Admissible constant
B	Batch number
F	Input feature number
$p(\mathbf{x})$	Synthetic data probability Distribution
C_0	Uplifted dimension
\mathbb{D}_m	Detail spaces
\mathbb{A}_m	Approximation space
\oplus	Orthogonal sum
J	Number of iterations
\mathbf{r}	Output probabilities
μ_s	Mean
σ_s	Standard deviation
Q	Original dimensions
O	State transition probabilities
p	Actual number of variable
W	Weight matrix
B	Observation probability distribution
d	Latent Variable dimension
π	Initial probability of a hidden state
M	Covariance Matrix

C_y	Critic Network
s	Standard deviation
γ_X	Xenon yield per fission
S	Covariance Matrix
γ_I	Iodine yield per fission
α	Confidence limit
λ_I	Xenon decay
D	Diffusion constant
λ_X	Iodine decay constants
ν	Thermal neutron speed
$M1$	Static Mode 1
$M2$	Static Mode 2
$M3$	Static Mode 3
X	Input Data Matrix
l	Prompt neutron lifetime
A_{ij}	Area of interface
$T1$	Transitional Mode 1
V_i	Volume of i^{th} zone
$T2$	Transitional Mode 2
q_t	Hidden state at time t
μ	Mean
$\hat{\boldsymbol{x}}$	Synthetic Data
$p(\boldsymbol{x})$	Synthetic Data Probability Distribution
β	Total delayed neutron fractional yield
T_{ci}	Global monitoring statistics
X_i	Distance between the centers of nodes
\mathcal{W}_{up}	Forward uplifting wavelet Transforms
\mathcal{W}_{down}	Downlifting wavelet transforms