Quantum computing assisted deep learning for fault detection and diagnosis in industrial process systems

Abstract:

Recent years have witnessed a surge in the intersection of quantum computing (QC) and deep learning, leading to innovative research. This study introduces a pioneering method that unites quantum computing with deep learning techniques to confront computational challenges that have historically impeded conventional approaches on classical computers. The proposed model makes use of deep belief networks to extract multi-tiered features from both normal and faulty processes. The approach combines quantum-enhanced generative training with discriminative training, successfully overcoming the limitations of traditional methods. When put in to the monitoring of the CSTR and the Tennessee Eastman (TE) process, this quantum computing-based method demonstrates strong and reliable performance. To be more specific, it achieves a mean fault detection rate of 79.2% for CSTR and an impressive 99.39% for TE.

Introduction:

The field of fault detection and diagnosis in process systems engineering has gained significant attention due to the increasing need for safe and efficient industrial operations. The potential risks associated with accidents in chemical plants, which can have widespread environmental and economic impacts, emphasize the importance of robust process monitoring. Multivariate statistical process monitoring, a data-driven technique, has become popular for its ability to utilize historical process data without requiring an in-depth understanding of the underlying physical models, making it a practical choice for process control.

Quantum computing (QC) is a revolutionary technology known for its applications in optimization, molecular design, and process scheduling. Despite the inherent quantum randomness and uncertainty due to factors like magnetic fields and thermal fluctuations, these traits can be leveraged to create efficient statistical machine learning methods. QC-boosted machine learning techniques have demonstrated significant potential across diverse applications, including data fitting and quantum recommendation systems. Their promise shines particularly bright in the realm of fast and accurate fault detection in process control.

However, the complete implementation of quantum computing-based methods faces obstacles due to the constraints of commercially accessible quantum computers, such as a deficiency of quantum bits (qubits), restricted connectivity, and the absence of quantum memory. To tackle these issues, scientists are investigating a holistic strategy that merges QC-boosted learning approaches with conventional machine learning algorithms.

To tackle these challenges, this research presents a pioneering strategy that merges quantum computing with deep learning to enhance the capabilities of fault detection and diagnosis. It employs deep neural architectures founded on Restricted Boltzmann Machines (RBMs) to efficiently extract features from both normal and faulty process operations. A significant breakthrough lies in the quantum-assisted training algorithm, which mitigates the computational complexities typically associated with training RBMs. The efficacy of this method is exemplified through practical case studies involving the CSTR and the Tennessee Eastman (TE) process, underscoring its suitability for intricate industrial contexts.

In summary, this research bridges the realms of quantum computing and deep learning to elevate fault detection and diagnosis in intricate process systems. By harnessing the strengths of both approaches, it offers a promising solution to real-world challenges in industrial settings.

Background:

Adiabatic quantum computing (AQC) stands out as a pivotal quantum computing model primarily designed to tackle optimization problems. AQC exploits the phenomenon of quantum tunnelling to explore and converge towards optimal solutions, often reaching the global minimum. This process surpasses the capabilities of classical methods like simulated annealing and goes by the name "adiabatic quantum optimization" (AQO). Unlike stochastic approaches, AQC offers a more sophisticated method for escaping local minima.

The core concept of AQC revolves around the step-by-step shift from a low-energy eigenstate of the initial Hamiltonian to the ground state of the ultimate Hamiltonian. These Hamiltonians serve as mathematical descriptions of energy in physical systems and are akin to the objective functions in optimization problems. AQC employs an adiabatic optimization process, guiding the progressive transformation of the quantum state toward the specified target problem Hamiltonian while reducing the influence of the initial Hamiltonian. This evolution is controlled by the magnitude of the initial Hamiltonian.

To employ AQC for optimization tasks, these problems must be reformulated into Ising models or quadratic unconstrained binary optimization (QUBO) problems. Quantum processors available in the commercial domain, like those from D-Wave Systems, are tailored for AQO. These processors employ a qubit lattice interconnected following a Chimera graph pattern. Translating the objective function onto this lattice demands a process referred to as minor embedding.

In practice, the performance of AQC systems is significantly impacted by the presence of noise. Various factors such as thermal fluctuations, internal quantum noise, and external noise sources can influence the outcomes of AQC operations. Noisy qubits may steer the system away from globally optimal solutions, thus affecting its optimization performance. Nonetheless, this noise can be harnessed for applications in machine learning, particularly for approximating sample distributions to model data distributions.

While AQC offers quantum advantages, its role in process systems engineering has yet to be fully established. Another central concept introduced in the text pertains to Restricted Boltzmann Machines (RBMs). RBMs are stochastic artificial neural networks with a generative nature, commonly used to model and analyse data distributions. They have found applications in diverse fields like image generation and recommendation systems. RBMs comprise visible and hidden units, forming an undirected bipartite graph connected by weights and biases. These RBMs play a crucial role in deep learning and feature extraction, aiming to optimize the likelihood of observed data. Training RBMs typically involves the application of the Contrastive Divergence (CD) learning algorithm, which approximates model expectations by running a Gibbs chain for k steps, making training computationally feasible.

An adaptation of RBMs enables them to handle real-valued data by replacing Bernoulli visible units with Gaussian visible units, widening their range of applications. Moreover, deep architectures known as Deep Belief Networks (DBNs) are constructed by stacking RBM layers. DBNs offer multi-level feature extraction capabilities and are trained in a layered, stepwise manner.

In conclusion, AQC and RBMs represent significant advances in the realms of quantum computing and machine learning. AQC holds the promise of revolutionizing optimization problems, while RBMs and DBNs serve as versatile tools for modelling data distributions and extracting features. A comprehensive grasp of the principles and applications of these concepts is essential to harness their potential across various domains, ranging from quantum computing to deep learning and data analysis.

Methods:

The novel approach for diagnosing faults in industrial processes employs a unique two-step methodology that combines the strengths of quantum computing (QC) and deep learning techniques. This fusion involves quantum generative training and supervised discriminative training, incorporating class labels, all aimed at enhancing the accuracy of fault detection.

In the initial phase, two distinct Deep Belief Network (DBN) sub-networks, specifically DBN-N and DBN-F, come into play for feature extraction from historical process data encompassing both normal and faulty states. The rationale behind deploying these two separate DBN sub-networks lies in accommodating the inherent variations in feature extraction from each sub-network. This approach inherently yields more dependable outcomes compared to a single DBN, thanks to its superior feature extraction capabilities. The amount of training data needed depends on model complexity and the training algorithm intricacies. A common guideline suggests having a dataset size at least ten times larger than the number of input dimensions. Analysing the relationship between dataset size and model performance helps determine the right dataset size for the desired level of accuracy.

In the subsequent step, the amalgamated features extracted from the DBN sub-networks constitute the input for a local classification sub-network. This sub-network's core function revolves around predicting the state of the initial input data vector, distinctly classifying it as either normal or faulty. This stage aligns with a supervised discriminative learning approach, incorporating class labels as an additional output layer.

The quantum generative training process initiates with the utilization of two DBN sub-networks designed for feature extraction. Each DBN sub-network consists of a pair of Sequential Restricted Boltzmann Machines (RBMs) stacked sequentially. These RBMs are well-suited for processing inputs with continuous values. The initial RBM layer features Gaussian visible units and Bernoulli hidden units, while the second RBM layer employs Bernoulli units for both its visible and hidden layers. Quantum sampling is systematically used to estimate model expectations, with a crucial parameter, βeff, influencing this process. The RBMs' parameters undergo iterative updates with a focus on minimizing the reconstruction loss between the input and the reconstructed data vectors. The outcome of this quantum generative training process is a higher-level abstraction of historical process data, serving as input for the subsequent classifier.

As for discriminative training, the elevated-level abstractions originating from the DBN-N and DBN-F sub-networks are concatenated and collectively serve as input for the local classifier. The local classifier exhibits the architecture of a neural network, proficiently predicting the probabilities associated with normal and faulty states. This network configuration incorporates fully connected layers alongside a SoftMax layer. The model parameters are meticulously fine-tuned by employing the backpropagation algorithm in adherence to a supervised learning paradigm. The essence of this training process revolves around the minimization of the categorical cross-entropy loss, an endeavour that ensures maximum likelihood parameter estimation.

In the final version of the model, the DBN-N sub-network undergoes a one-time training phase and can be efficiently applied to multiple diagnostic processes. When it comes to determining the state of a new process data sample, the abstractions derived from both normal and faulty states, generated by the DBN-based generative model, are thoughtfully fused. At this juncture, the local classifier comes into play, offering its predictions in the form of probabilities that indicate whether the sample should be classified as normal or faulty. This classification is substantiated by implementing a threshold probability of 0.5, finalizing the data sample's categorization.

In summation, this innovative two-step approach seamlessly marries quantum generative training with classical discriminative training, presenting a potent framework for advancing fault diagnosis within industrial processes. It harnesses the prowess of quantum computing to augment feature extraction capabilities and, in turn, the overall accuracy of the diagnosis process.

CSTR:

In a real-world application, a group of researchers carried out experiments involving a Continuous Stirred Tank Reactor (CSTR), an apparatus designed to emulate chemical reactions and gather data on various parameters. Their primary goal was to devise a method capable of identifying irregularities or issues within the reactor's functioning. The study encompassed three distinct types of simulated faults: issues related to sensor functionality, declines in catalyst activity, and the accumulation of impurities in the cooling system.

The research leveraged data stemming from both the routine and faulty operations of the reactor to facilitate the training of a pioneering quantum computing-driven model for the purpose of fault detection. This groundbreaking model delivered an impressive performance, accurately flagging faults in the reactor with a notable precision rate of 86.08%. It's worth emphasizing that this level of accuracy outshone traditional methodologies typically applied for similar fault detection tasks.

Nevertheless, it's crucial to acknowledge that the model did exhibit a false alarm rate of 19.41%. This implies that, in certain instances, it erroneously identified issues even when none were actually present. While this false alarm rate represents a noteworthy limitation, the study underscores the substantial potential of merging quantum computing and deep learning techniques to enhance the detection of faults within intricate systems, such as the CSTR.

To sum it up, the research initiative involved a series of experiments conducted with a CSTR, focusing on the identification of operational anomalies and issues. A quantum computing-based model was meticulously trained using data originating from both normal and faulty operations, yielding a remarkable 86.08% accuracy in the realm of fault detection. Despite the existence of a 19.41% false alarm rate, the study effectively spotlights the promising outlook for harnessing quantum computing and deep learning to advance the fault detection capabilities in complex systems akin to the CSTR.

Tennessee Eastman Process:

The Tennessee Eastman (TE) process, outlined in Downs and Vogel's work from 1993, stands as a well-established benchmark in the realm of process monitoring. It serves as a rigorous litmus test for evaluating innovative monitoring techniques. This intricate chemical process involves the production of two primary products and encompasses five significant process units: a reactor, stripper, separator, compressor, and mixer. The TE process simulation includes a grand total of 52 variables, consisting of 41 measured variables and 11 manipulated variables. To thoroughly challenge the proposed Quantum Computing (QC)-based fault detection model, the TE process introduces a complex scenario with 20 distinct fault states in addition to the normal operating state. Each fault state yields 1,200 data samples, gathered at three-minute intervals over a 75-hour duration.

Every fault is deliberately injected into the system following a continuous 10-hour period of normal operation. As a result, the initial 200 samples within each dataset exhibiting faults depict the typical operation of the process, while the subsequent 1,000 samples capture the manifestation of faulty conditions. In contrast, the dataset representing normal processes encompasses uninterrupted data collected over a span of 48 hours. To conduct a comprehensive evaluation of the QC-based fault diagnosis model's performance for both normal and faulty states, a distinct testing dataset was meticulously recorded, featuring 600 samples gathered over a 30-hour duration, with faults introduced after 10 hours of uninterrupted normal operation.

To mitigate the variance associated with Gaussian noise in the visible units, the data from both normal and the 20 faulty states were normalized to exhibit a zero mean and unit variance. All 52 process variables were retained as inputs for the proposed model without any elimination, highlighting the model's capability to effectively handle extensive and intricate datasets.

Both the DBN-N and DBN-F sub-networks were designed with an identical architecture to create abstractions for normal and faulty states. In the initial RBM layer of these sub-networks, there were 52 visible Gaussian units and 26 hidden Bernoulli units, resulting in an output generated through a simple perceptron operation. The subsequent RBM layer was equally intricate, composed of 26 visible units derived from the hidden units in the previous layer, along with an additional 20 hidden units, producing an output using binomial distribution-based sampling. Quantum generative training was carried out for these DBN sub-networks, with specific parameters, including a learning rate set at 0.01 and a constant momentum value of one. The outputs from these DBN-based sub-networks were combined into a 40-dimensional data vector, which played a crucial role in the discriminator sub-network. This discriminator sub-network featured a fully connected layer housing 40 neurons. Fine-tuning was a meticulous process, involving the training of the discriminator using the Adam optimizer, with a particular emphasis on minimizing categorical cross-entropy loss.

The quantum generative training procedure made use of an adiabatic quantum computer (AQC) for quantum sampling, enabling the estimation of model expectations. In this process, the D-Wave 2000Q quantum processor was employed, equipped with an impressive array of 2,048 qubits and 5,600 couplers. These quantum resources were accessible through a cloud-based remote operation framework. Each computational run adhered to a carefully designed anneal schedule, with a fixed duration of 20 microseconds (20μs). To maintain consistency and facilitate the effective management of the temperature-dependent parameter, denoted as βeff, an embedding scheme tailored to the energy function of each Restricted Boltzmann Machine (RBM) instance was thoughtfully established. It's noteworthy that βeff was intentionally set to a unity value to simplify the model.

A local classifier was enlisted for fault detection, determining the Fault Detection Rates (FDR) and False Alarm Rates (FAR) for each fault, classifying data samples as normal or faulty using a threshold probability of 0.5. The results exhibited an average FDR of 99.39%, coupled with an impressively low FAR of merely 5.25%, signifying the high efficiency of the fault detection model with minimal false alarms.

Moreover, a global classifier network was introduced to specifically identify the types of faults, with an output probability assigned to each fault type, serving as input for the global classification network. The global classifier remarkably outperformed other fault diagnosis models, demonstrating the QC-based model's superiority. For instance, it achieved an FDR of 44.9% for a particularly challenging fault (Fault 15), surpassing the performance of alternative models.

The study also conducted an evaluation of performance using a confusion matrix, offering a visual representation of classification accuracy and misclassification. The matrix unveiled notably high detection rates for several fault types, especially those with distinctive characteristics. Even the lowest FDR observed for Fault 9 stood at 38.1%, underscoring the model's proficiency in effectively distinguishing between different fault types.

To conclude, this study vividly showcases the potential of a Quantum Computing-based model for fault detection and diagnosis within complex chemical processes. The model attains a remarkable level of detection accuracy while maintaining an impressively low rate of false alarms, signifying its promise for practical applications in the domains of process monitoring and fault detection.

Quantum Advantage:

Classical training techniques for Deep Belief Networks (DBNs) typically involve approximating the log-likelihood gradients of training data, often using the Contrastive Divergence (CD-k) algorithm. Yet, CD-k comes with its constraints since it doesn't adhere to a particular function's gradient and mandates multiple iterations to achieve convergence due to the influence of noise in Gibbs sampling. In contrast, quantum generative training offers a solution to some of these challenges. It quantifies a quantum advantage in terms of computational effort and time required to achieve a specific model performance. You can compare quantum training to classical techniques by examining the loss curves of RBM layers in the DBN-F sub-network. The quantum approach demonstrates faster convergence, representing a quantum advantage. Importantly, the computation time required for quantum techniques is negligible and doesn't increase with network size, making it especially advantageous for larger networks.

In the case of complex process systems, such as those analysed in the study, it shows high detection rates and fewer false positives. This model can be applied broadly to nonlinear complex process systems with minimal adjustments. Quantum advantages, including faster convergence and computational speed, provide a competitive edge, particularly as the number of process variables increases.

In conclusion, quantum generative training offers a more efficient and rapid training approach for DBNs compared to classical methods, making it particularly valuable in complex systems where accuracy and speed are essential.

Conclusions:

This research presents an innovative quantum-powered approach for fault diagnosis in intricate industrial processes. By integrating quantum generative training with classical discriminative training, we aimed to enhance the detection and diagnosis of various faults. The model underwent rigorous testing on two distinct industrial processes, surpassing the performance of established methods. This highlights the promising potential of quantum computing in advancing fault diagnosis within industrial settings.