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Generative Adversarial Networks (GANs) Applications in Chemical Engineering

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Abstract: *In the field of machine learning, Generative Adversarial Networks (GANs) have arisen as an influential tool demonstrating exceptional capabilities in generating synthetic data that closely comply with real-world samples. The last decade has seen remarkable advances in speech, image and language recognition tools that have been made available to the public through computer and mobile devices' ap-plications in broad area of sciences, including Chemical Engineering. In this pa-per, existing and future potential applications of GANs in Chemical Engineering have been given in detail. GANs have a strong potential to revolutionize in chem-ical engineering and its multiple subfields such as process optimization, molecular design, and materials science. Based on the searches on recent literature and case studies, generating realistic molecular structures, fault diagnosis and predicting chemical properties, optimizing process parameters, and designing novel materi-als are some of the GANs applications in chemical engineering. Challenges and opportunities associated with the integration of GANs into traditional chemical engineering workflows have also been discussed. Additionally, future potential applications of GANs have been examined with examples, in this paper.*

Keywords: *Generative Adversarial Networks, Artificial Intelligence, Chemical Engineering.*

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I. INTRODUCTION

Generative Adversarial Networks, or GANs for short, are an approach to generative modeling using deep learning methods, such as convolutional neural networks. Generative modeling is an unsupervised learning task in machine learning that involves automatically discovering and learning the regularities or patterns in input data in such a way that the model can be used to generate or output new examples that plausibly could have been drawn from the original dataset. GANs are a class of Deep Neural Networks that have the ability to generate realistic synthetic data including but not limited to images, text, or even videos. As a result of these revolutionary developments, Generative AI is transforming the field of chemical engineering, enabling researchers and engineers to achieve higher levels of efficiency, reduce costs, and drive innovation in the chemical industry. Generative Adversarial Networks (GANs) is one of the most popular approaches used in Generative AI, providing researchers with a powerful tool for designing novel chemical compounds, optimizing process parameters, and designing innovative materials.

A GAN uses a decoder (or generator) and discriminator to learn the materials data distribution implicitly. In GAN approaches, a key component of crystal structural generative models is the invertibility from material representation (features) to real structure of material since the features generated from the latent vector should eventually be inverted back to the real structure of material in order to confirm the generated material [1, 2]. A generative adversarial network (GAN) employed for crystal structure generation using a coordinate-based crystal representation inspired by point clouds [3]. By conditioning the network with the crystal composition, the proposed model generated materials with a desired chemical composition. As an application in this model, GAN architecture applied to generate new Mg−Mn−O ternary compounds to find potential photoanode materials and discovered 23 new crystal compounds with reasonable stability in an aqueous environment and band gap.

Stacked denoising autoencoders (SDAE) combined with GAN for planetary gearbox fault pattern recognition with limited fault samples and strong noise interference [4]. An auxiliary classifier GAN (ACGAN) model developed to learn from mechanical sensor signals and generate realistic one-dimensional raw data and used a CNN classifier to output the machine fault diagnosis result [5]. A supervised classifier framework with GAN introduced to increase the number of faulty training samples and re-balance the training dataset and performed robust fault diagnosis for air handling units [6]. An enhanced ACGAN built with deep neural network (DNN) to solve imbalanced problems and classify the chemical process faults [7]. A high-efficiency GAN model (HGAN) proposed for chemical process fault diagnosis [8]. HGAN integrates the advantages of Wasserstein GAN

and Auxiliary Classifier GAN to promote the generating model training stability and the discriminative model training efficiency with Bayesian optimization.

A vast number of organic molecules are applied in solar cells, such as organic light emitting diodes, conductors, and sensors [9]. Synthesis of new organic and inorganic compounds is a challenge in physics, chemistry and in materials science. A number of machine learning approaches were proposed to facilitate the search for novel stable compositions [10]. There was an attempt to find new compositions using an inorganic crystal structure database, and to estimate the probabilities of new candidates based on compositional similarities. A learning method called CrystalGAN proposed to discover cross-domain relations in real data, and to generate novel structures [11].

Near-infrared (NIR) spectroscopy has been widely used to predict the chemical properties of materials especially gasoline properties that are difficult to measure online during gasoline blending. NIR models should be prepared in advance to apply this technique successfully. Obtaining a high-accuracy NIR model in practice is hard because abundant labelled samples are difficult to acquire. The application of WGAN presented for the prediction of octane number by NIR spectroscopy. It is observed that when labelled data are insufficient during gasoline blending, the proposed method can help to establish an initial NIR model quickly [12].

In this paper, detailed literature search results have been given for the main application areas of Generative Adversarial Networks on Chemical Engineering. The main aim of this work is to provide a milestone point to the reseachers who want to apply GANs to their future researches in Chemical Engineering area.

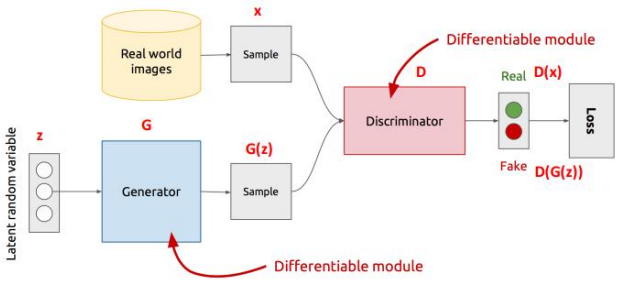
II. GANs APPLICATIONS IN CHEMICAL ENGINEERING

Detailed representations of three different GANs applications have been given in detail.

1.1 Generative Adversarial Networks (GANs).

In 2014, a groundbreaking paper by Ian Goodfellow et al. introduced the world to Generative Adversarial Networks (GANs). As depicted in Fig. 1, this ingenious technique revolutionized the field of artificial intelligence by creating a system that pits two neural networks against each other. One network, the generator, strives to create ever-more realistic data, be it images, music, or even 3D models. The other network, the watchful discriminator, aims to distinguish the generated creations from real-world samples.

Figure1. GANs architecture.

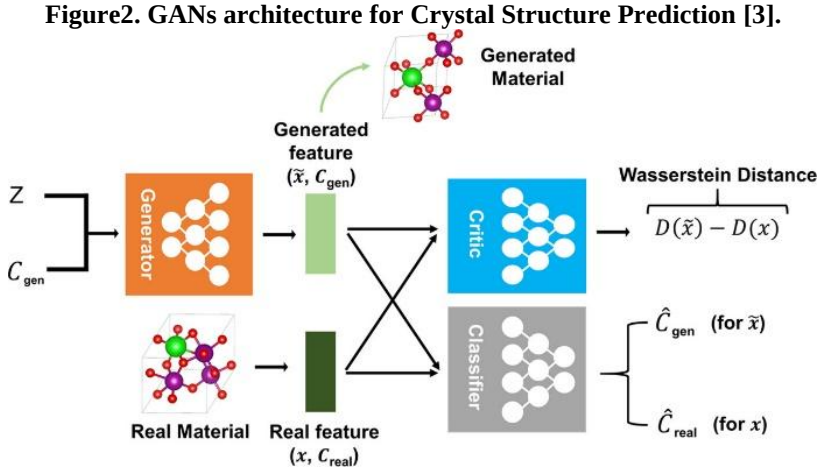


- **Z** is some random noise (Gaussian/Uniform).
- **Z** can be thought as the latent representation of the image.

1.2 Generative Adversarial Networks for Crystal Structure Prediction

One of the proposed GANs model [3] for Crystal Structure Prediction consists of three network components: a generator, a critic, and a classifier as shown in Fig. 2. The generator takes the random Gaussian noise vector (Z) and one-hot encoded composition vector (Cgen) as the input to generate new 2D-representations. The one-hot encoded composition vector is used as a condition to generate materials with target composition. The critic computes the Wasserstein distance which represents dissimilarity between the true and trained data distributions, and by reducing this distance the generator would generate more realistic materials. The critic network is composed of three-shared multilayers perceptions (MLPs) followed by average pooling layers to ensure the permutation invariance under the reordering of points in the 2D-representation. It is noted that the permutation invariance under the reordering of input is satisfied by using shared weight parameters and average pooling since the averaged value is unchanged under the change of orders. The classifier network, which outputs the composition vector from the input2D-representation, is used to ensure that the generated new materials meet the given composition condition. The loss of the classifier is back-propagated to the generator only if the generated 2D-representation ($\tilde{x}$) is taken as input.

Figure2. GANs architecture for Crystal Structure Prediction [3].

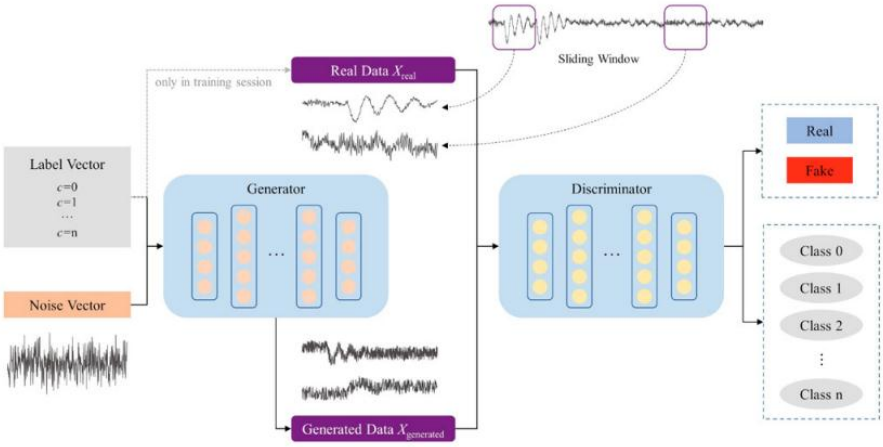


Z, Cgen, and Creal denote a random input noise, user-desired composition condition, and composition of real material, respectively. The variables x̃ and x denote the feature (representation)of generated and real materials, respectively. Ĉgen and Ĉreal denote the predicted composition of the generated and real features, respectively. D(x) is the critic function also known as the critic network.
As an application in this model, GAN architecture applied to generate new Mg−Mn−O ternary compounds to find potential photoanode materials and discovered 23 new crystal compounds with reasonable stability in an aqueous environment and band gap.

1.3 **Application of GANs In Chemical Process Fault Diagnosis**

Another one of the proposed GANs model used to fault diagnosis in a chemical process [8]. As given in Fig. 3., the proposed HGAN model incorporates the advantages of WGAN and ACGAN, which utilizes Wasserstein distance and gradient penalty to empower the generator training process, and adopts the Bayesian optimization strategy to enhance the discriminator performance.

Figure3. ACGAN (HAGN) model structure for fault diagnosis.

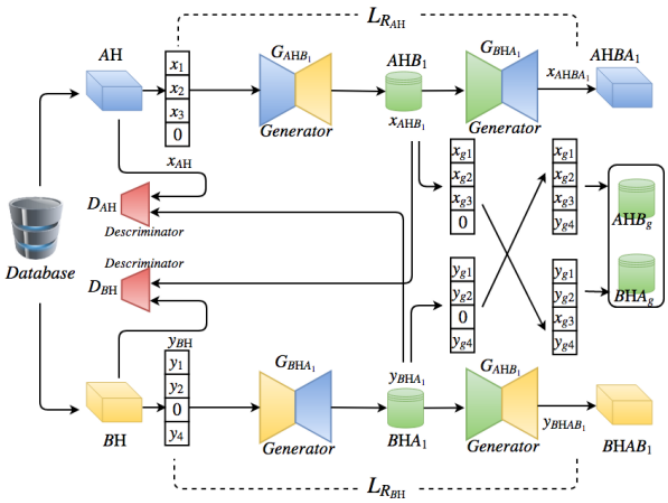


At the offline stage, raw data of the chemical process is collected including operation parameters and process parameters, which is subsequently divided into different sets for training and testing. After normalization and other necessary preprocessing steps, the training dataset is used to train the HGAN model and acquire the optimized parameters of the generator and the discriminator. The benchmark Tennessee Eastman process (TEP) simulator is applied to evaluate the performance of the proposed model. The experiments are conducted with small size of training samples under data balance and data imbalance conditions separately. The diagnosis results of HGAN are compared with a traditional statistical model.

1.4 **Learning to Discover Crystallographic Structures with GANs**

As the last example, a CrystalGAN [11] which generates new chemically stable crystallographic structures with increased domain complexity will be given. The basic architecture of the CrystalGAN presented in Fig. 4.

Figure4. CrystalGAN model architecture for discovering crystallographic structures.



In this work [11], authors focus on applications of hydrogen storage, and in particular, the problem to investigate novel chemical compositions with stable crystals. Based on the CrystalGAN model architecture for discovering crystallographic structures, it is noted that although the CrystalGAN was developed and tested for applications in materials science, it is a general method where the constraints can be easily adapted to any scientific problem.

III. CONCLUSION

Generative Adversarial Networks (GANs) have emerged as a powerful tool for Chemical Engineering, offering a glimpse into a generative future. Their ability to create realistic and intricate data holds immense potential for accelerating material discovery, optimizing processes, and empowering data-driven approaches. While challenges like data scarcity and model interpretability remain, advancements in machine learning and computational resources promise even more sophisticated applications in the coming years. By embracing GAN technology, Chemical Engineering can unlock entirely new avenues for innovation, leading to a more sustainable and efficient future for the industry.

Conflict of interest

There is no conflict to disclose.

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