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Quantum-Based Prediction Model for Carbon Neutrality

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***Abstract*—Carbon neutrality is a global target pursued by cities worldwide to achieve a balance between carbon emissions and removals, reaching a net-zero carbon state. Mitigation measures are being implemented to reduce emissions and enhance carbon sequestration, aiming to meet the targets set for 2050 or 2060. However, challenges posed by urban sprawl and increasing urbanization raise concerns about the feasibility of achieving carbon neutrality. Various studies have been conducted to project the attainment of this goal by developing prediction models. Machine learning (ML) prediction models use socio-economic, energy, and technological data to forecast carbon neutrality. These models consider factors like GDP per capita, urbanization rate, total energy consumption, and forest stock volume, formulating scenarios based on policy documents and historical data. Some models have incorporated optimization methods like the sparrow search algorithm, genetic neural network, and aquila optimizer to improve prediction accuracy. However, classical optimization methods have limitations, such as susceptibility to getting trapped in local optima, which can affect model performance. Quantum-based optimization methods, particularly quantum annealing (QA), are emerging as potential solutions to address these challenges by leveraging the principles of quantum mechanics to optimize complex problem spaces. QA enhances ML processes like feature selection, hyperparameter optimization, and regression model optimization. This study provides a review of pipeline processes from state-of-the-art methods, as well as their potential quantum-based enhancements, to achieve more precise predictive models.**

Keywords—Prediction Model, Carbon Neutrality, Machine Learning (ML), Quantum Annealing (QA)

I. INTRODUCTION

Carbon neutrality, the goal of achieving a balance between carbon emissions and removals to reach net-zero carbon, is being pursued by cities worldwide [1],[2]. Human activities in urban areas, including energy usage, transportation, waste management, and land use, directly and indirectly impact carbon emissions [3]. Many countries have set specific targets to achieve carbon neutrality by 2050 or 2060, with carbon peak times centered around 2030 [4]–[8]. To meet these targets, various efforts and mitigation measures have been implemented [9], including reducing carbon emissions and increasing carbon sequestration. However, challenges such as urban sprawl and the trend of urbanization pose obstacles to this progress [10]. As a result, there are concerns about whether the vision of carbon neutrality can be achieved or if it will remain an aspiration.

Several studies have developed ML prediction models to assess the attainment of carbon neutrality using socio-economic, energy, and technological data [4]–[8]. These models consider factors such as GDP per capita, urbanization rate, total energy consumption, and forest stock volume as predictors of carbon emissions and sinks. Additionally, various scenarios based on policy documents and historical development levels have been formulated to measure future progress towards carbon neutrality. Successfully achieved scenarios include the green development scenario [7], adjusting electricity emission intensity [5], low energy demand with multiple treatments [8], and the high-enhancement scenario [4]. The findings of these studies provide valuable policy recommendations, such as improving energy utilization efficiency, developing carbon removal technologies, managing population, and controlling total energy consumption [4]–[8].

While classical optimization methods like the sparrow search algorithm [7], elastic net regression [5], genetic neural network [8], and the aquila optimizer [4] are still commonly used to enhance ML predictions, they have limitations in optimization. These limitations include being prone to getting trapped in local optima and being unable to guarantee global optima [11], which can impact the quality of solutions obtained. Consequently, there is a growing interest in utilizing quantum-based optimization methods, such as QA [11], [12], to improve ML. QA can be employed for various ML optimization processes, including training, prediction, classification, clustering, and neural network optimization.

Unlike classical approaches that rely on classical mechanics, quantum-based approaches utilize the principles of quantum mechanics, including quantum bits (qubits), superposition, and inference. These approaches have the ability to overcome the limitations of conventional computing, which is crucial for obtaining optimal solutions in complex problem spaces [11]. Quantum-based approaches are commonly used to solve optimization problems such as NP-hard and probabilistic sampling [11], [13]. However, in the context of this study, the current state-of-the-art methods still rely on classical ML. By integrating quantum-based approaches with ML, it is possible to enhance predictive models and produce better results. This study aims to integrate quantum-based approaches with ML to create an optimal carbon neutrality prediction model. The integration of ML with quantum approaches offers several advantages, including optimized feature selection, accelerated hyperparameter optimization, and streamlined regression model optimization [12]. Therefore, this paper proposes two main contributions: (1) a carbon neutrality prediction model framework developed by state-of-the-art methods, and (2) the enhancement of ML

prediction models using quantum-based methods to improve predictive accuracy.

Section II provides background information, Section III reviews relevant previous research, Section IV explains the quantum-based prediction model, and Section V presents the conclusions and future directions of this study.

II. Background

A. Carbon Emissions

The calculation of carbon emissions from various sources follows the established formulation in the global protocol for greenhouse gas inventory [14], with the following equation:

$$C_e = \sum_{i=1}^{n} AD_i \; . \; EF_i \tag{1}$$

where C_e is the total carbon emissions, AD represents activity data in quantitative form, and EF is the carbon emission factor. Generally, carbon emission inventories involve several key sources, such as energy, transportation, industrial processes, land use, and waste.

B. Carbon Sinks

Carbon sink in urban areas is calculated based on the vegetation in green open spaces using the following equation [15]:

$$C_s = LA \cdot S \tag{2}$$

where C_s is the carbon sink capacity based on green open spaces, LA is the area of green open space (m^2), S is the carbon sequestration rate ($\mu g/m^2/year$) given by $0.2278e^{(0.0048 \cdot I)}$, with I representing light intensity (kal/cm^2/day).

C. Carbon Peak

Carbon peak refers to the point in time when a country's carbon dioxide (CO_2) emissions reach their highest level before starting to decline. Most countries have set targets to achieve carbon peak around the year 2030 [4], [16].

D. Carbon Neutrality

Carbon neutrality refers to the achievement of a state in which there is a balance between carbon emissions and carbon absorption from the atmosphere. The goal is to have net-zero carbon, meaning the amount of CO_2 emitted is offset by the amount removed [4], [7]. The formula for measuring carbon neutrality is as follows:

$$C_n = C_e - C_s \tag{3}$$

where C_n is the total remaining carbon after substracting C_s from C_e. An area is considered carbon neutral if $C_n \leq 0$.

E. Quantum Annealing (QA)

The quantum gate model and QA differ significantly in their implementation and offer unique benefits compared to classical computing. The gate model tackles problems by breaking them down into a series of basic operations (gates) that yield clearly defined "digital" measurement outcomes, similar to classical computing. On the other hand, QA effectively samples low-energy configurations of quantum systems and excels in solving optimization problems, including NP-hard, combinatorial, and probabilistic sampling problems [11], [17].

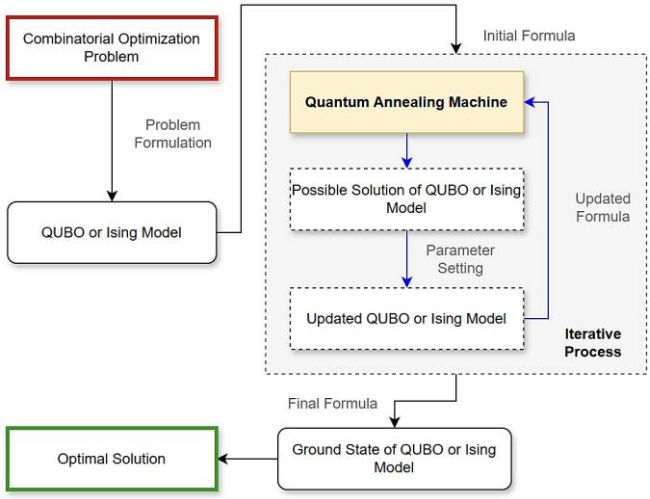

Fig. 1. Combinatorial optimization problem utilizing quantum annealing machines (adopted from [17])

Fig. 1 shows the process of solving optimization poblem using QA machines. QA operates via a quantum adiabatic process, beginning with the preparation of the ground state using the Initial Hamiltonian. It then evolves adiabatically until it transforms into the Final Hamiltonian, which represents the optimal solution to the problem. QA machines solve large-scale optimization problems by converting them into quadratic unconstrained binary optimization (QUBO) or Ising models with mathematical representation. The following equation is the formulation of QUBO [18]:

$$E(x_i) = \sum_{i,j} A_{i,j} x_i x_j \tag{4}$$

where $x_i \in \{0,1\}$ is the binary decision variable of problem, and $A_{i,j} \in \mathbb{R}$ are the coefficients.

III. Related Works

A. Prediction Models for Carbon Neutrality

1) Dataset

The datasets used to predict carbon neutrality come from various sources, including energy, socio-economic, carbon emissions, and climate data. These datasets represent both direct and indirect factors that influence carbon emissions projections for the future. Carbon emissions in a specific area can be calculated using Equation 1, while reduction factors such as the area of green open spaces can be calculated using Equation 2. In one study [8], diverse datasets such as C-GEM, MESSAGEix, GAINS, and CE3METL energy models, along with Shared Socio-Economic Pathways (SSPs), were used. Another study [5] relied on a crucial dataset that included building-level electricity consumption in Hong Kong for over 39,000 buildings from 1982 to 2016. This dataset was supplemented with additional variables such as temperature,

construction details, socio-economic factors, and local climatic conditions. Studies [4] and [7] used national and international datasets that provide information on GDP, population, urbanization, energy consumption, and carbon emissions. Similarly, study [6] used historical data on China's carbon emissions from 1990 to 2018 as the basis for future projections. Selecting appropriate datasets is crucial in developing accurate prediction models.

2) Feature Extraction

Feature extraction is important for identifying key factors, reducing data redundancy, and filtering out irrelevant criteria. The study [8] used different methods for feature extraction. For energy structure (ES), energy intensity (EI), and industrial structure (IS), they used partial least squares (PLS) regression, while linear regression was used for economic output (EO) and population (P) due to their one-dimensional inputs. The logarithmic mean divisia index (LDMI) model was used to decompose driving factors related to CO_2 emissions, considering variables such as P, per capita GDP, EI, and carbon intensity. This helped identify the contributions of different factors to total emissions. In study [5], the STIRPAT model and machine learning regression (MLR) techniques like least absolute shrinkage and selection operator (LASSO), Elastic Net, and Ridge regression were combined to select relevant factors and establish their historical correlation with building energy consumption. The MLR approach addressed issues of multicollinearity and overfitting. Study [7] used IPAT and STIRPAT to determine influencing factors, considering environmental impact, population, affluence, and technology levels as key factors. Gray relation analysis (GRA) was also used to handle complex problems involving multiple factors and nonlinear relationships, helping to understand the relationship between different factors and their impact on the target variable. Other methods for feature selection included LASSO, bayesian information criterion (BIC), and principal component analysis (PCA) as used in study [6]. LASSO extracted important information from various influencing factors, BIC guided the inclusion or exclusion of variables in a model, while PCA extracted features of the remaining variables to avoid missing information caused by feature selection.

3) Prediction Method

Previous studies have used various hybrid machine learning methods for predicting carbon neutrality. These include GRA-SSA-ENN [7], AO-ELM [4], DE-GWO-SVR [6], MLR [5], and ANN [8]. Study [7] employed the GRA algorithm to rank correlations and extract eight core elements as input variables for the prediction model, improving operational efficiency. The elman neural network (ENN) was used to handle dynamic temporal patterns, while SSA was utilized to optimize ENN parameters, addressing the issue of potential local optima. This optimization step ensures superior performance and accuracy. In study [4], the aquila optimizer (AO) was used to enhance the extreme learning machine (ELM) by finding optimal weights and thresholds. The AO technique simulates the hunting behavior of an aquila (eagle), involving steps to search and capture prey until the optimal solution is found. The AO-ELM model demonstrated better forecasting performance and lower simulation errors compared to traditional BPNN and single ELM models, indicating its effectiveness. Study [6] employed support vector regression (SVR) optimized with differential evolution-grey wolf optimization (DE-GWO). SVR excels with small sample sizes and avoids overfitting through a convex objective function. However, SVR's performance heavily depends on manually set and suboptimal initial parameters. DE-GWO was used to optimize SVR parameters, combining the strengths of DE and GWO to enhance the search for optimal parameters. DE effectively explores the search space, while GWO ensures convergence to the global optimum. Study [5] used MLR to forecast the carbon footprint by determining the historical correlation between building electricity consumption and its influencing factors. MLR also addresses potential multicollinearity and overfitting problems by selecting relevant variables and analyzing their correlations. Shrinkage methods like LASSO, Elastic Net, and Ridge regression were used. The results showed that MLR models demonstrated high accuracy in predicting electricity consumption, evidenced by the close match between estimated and reported values and high coefficients of determination (R^2). In another study, [8] used an artificial neural network (ANN) to predict driving factors of CO_2 emissions. The research utilized a multilayer feedforward neural network trained with the error back-propagation algorithm to forecast driving factors. The parameters of the carbon emission network were optimized using a genetic neural network in MathWorks MATLAB r2016a, achieving high accuracy and minimal error. Training performance was evaluated through mean square error (MSE), ensuring the artificial neural network (ANN) models delivered reliable predictions without overfitting. This thorough validation process was crucial in selecting the optimal networks for each driving factor.

4) Performance Measurement

Various evaluation methods, such as mean absolute percentage error (MAPE), mean absolute error (MAE), and root mean squared error (RMSE), can be used to measure the performance of predictive models. These indicators help gauge the discrepancy between actual values and predicted results. The lower the values of MAPE, MAE, and RMSE, the better the prediction model performs. The formulas for these indicators are provided below [7]:

$$RMSE = \sqrt{\frac{1}{T}\sum_{i=1}^{T}(y(i) - \hat{y}(i))^2} \quad (5)$$

$$MAPE = \frac{1}{T}\sum_{i=1}^{T}\left|\frac{y(i)-\hat{y}(i)}{y(i)}\right| \times 100\% \quad (6)$$

$$MAE = \frac{1}{T}\sum_{i=1}^{T}|y(i) - \hat{y}(i)| \quad (7)$$

where $y(i)$ is the actual value and $\hat{y}(i)$ is the predicted value.

5) Scenario Analysis

To effectively predict carbon emissions and achieve carbon neutrality, the study [4] proposes scenario analysis. The process begins by identifying key variables such as GDP per capita (GDPPC), urbanization rate (UR), and total energy consumption (TEC). Multiple scenarios are then developed based on different combinations of these variables, which reflect varying levels of economic growth, urbanization, and

energy consumption patterns. Each scenario incorporates different policy measures aimed at reducing emissions, enhancing carbon sinks, or promoting renewable energy sources to understand their impact on carbon emissions. Historical data is used to calibrate the models, ensuring that the scenarios are realistic and creating a baseline scenario that mirrors current trends and policies. Using these constructed scenarios, future carbon emissions and carbon sinks are projected over a specified period, taking into account potential carbon peaks. Prediction models are then applied to each scenario to forecast the future trajectory of carbon emissions and assess the effectiveness of different strategies. Finally, the outcomes of each scenario are evaluated by comparing the predicted emissions with the carbon neutrality targets, using Equation 3, to help identify the most effective pathways to achieve net-zero carbon.

B. Integrating ML with QA in Prediction Tasks

The integration of ML with QA has the potential to revolutionize computational methodologies, offering groundbreaking solutions for complex real-world problems and enhancing problem-solving capabilities. Classical ML demands extensive computational resources for parameter optimization due to the vastness of the solution space. In contrast, QA leverages quantum fluctuations to efficiently navigate these intricate spaces, providing accelerated solutions. The potential enhancements of ML through QA include [12]:

- Optimized Feature Selection: Feature selection is essential for model interpretability and performance, especially with high-dimensional datasets. QA offers a robust method to streamline this process by effectively exploring extensive feature spaces.
- Accelerated Hyperparameter Optimization: Hyperparameter optimization greatly impacts model performance, yet exploring large parameter spaces is computationally intensive. QA revolutionizes this process by simultaneously evaluating numerous hyperparameter settings.
- Streamlined Regression Model Optimization: Regression models used to predict carbon emissions, as seen in studies [5], [6], require precise parameter tuning, which is challenging in high-dimensional parameter spaces. QA addresses this by efficiently navigating parameter spaces, ensuring accurate predictions.

The fusion of QA with ML presents a transformative approach to computational challenges, promising enhanced efficiency, speed, and accuracy in various predictive tasks.

IV. The Quantum-Based Prediction Model

In developing a quantum-based prediction model, the framework is formulated by integrating steps from previous studies [4]–[8], as shown in Fig. 2. The model consists of three main phases: feature selection, model development, and carbon neutrality projection. Feature selection is the phase where the most suitable features are identified to be used as inputs for the prediction model. Model development involves constructing a prediction model with the highest possible accuracy through comprehensive evaluation. Finally, carbon neutrality projection is the phase where the achievement of carbon neutrality is projected under different scenarios to determine the optimal scenarios.

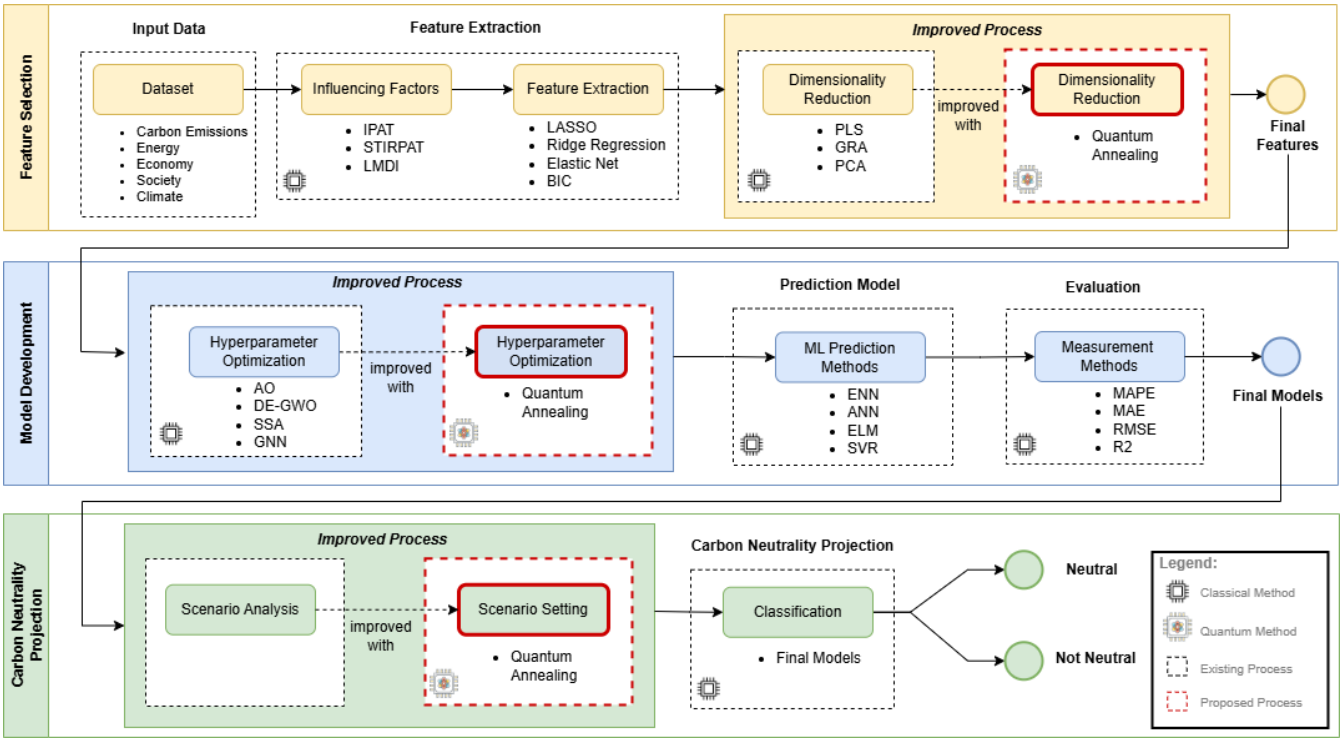

Fig. 2. Framework for carbon neutrality prediction models with quantum-based enhancements (combined from: [4]–[8])

Fig. 2 illustrates the stages of the overall prediction model, integrating various state-of-the-art methods utilized in previous studies along with proposed enhancements using quantum methods. The model combines classical and quantum approaches to optimize feature selection, hyperparameter tuning, and scenario analysis for predicting

carbon neutrality. The integration of quantum techniques, such as QA, aims to improve the efficiency and accuracy of the prediction model by effectively addressing combinatorial optimization problems compared to classical methods. The process begins with Feature Selection, which aims to identify and extract the most relevant features for the prediction model. It starts by collecting comprehensive dataset, including variables related to carbon emissions, energy, economy, society, and climate. Key influencing factors are identified using models like IPAT, STIRPAT, and LMDI. Feature extraction methods such as LASSO, Ridge Regression, Elastic Net, and BIC are employed to extract significant features. Dimensionality reduction techniques like PLS, GRA, and PCA streamline the feature set, and this process is enhanced by utilizing QA for more efficient reduction and final selection of features. Next is Model Development, which focuses on creating and optimizing the prediction model. Initially, hyperparameters are optimized using algorithms like AO, DE-GWO, SSA, and GNN. This process is improved the classical methods with QA for superior optimization results. Prediction models are developed using machine learning techniques such as ENN, ANN, ELM, and SVR. The models are then evaluated using metrics like MAPE, MAE, RMSE, and R^2 to ensure accuracy and reliability, resulting in the final models. Finally, in the Carbon Neutrality Projection phase, multiple scenarios are constructed and analyzed to predict future carbon neutrality outcomes. This process is improved by incorporating QA, enhancing the scenario setting process for more accurate and comprehensive analysis. The final models classify scenarios to project whether they will result in a neutral or non-neutral carbon status, providing valuable insights for stakeholders. Each of these improved processes is explained in the points below:

1) Dimensionality Reduction

Dimensionality reduction during feature selection is recognized as a combinatorial problem that can be effectively optimized using QA [19]. This problem must be converted into a format compatible with QA, such as the QUBO format. In this method, each feature's inclusion or exclusion is represented by binary variables, where "1" indicates the feature is selected, and "0" indicates it is not. The significance of each feature is evaluated based on its correlation with the target variable. QA's capability to find solutions without strictly enforcing constraints offers an advantage over classical techniques. The QUBO formulation seeks to identify the binary variable arrangement that optimizes the objective function, representing the subset of features that most effectively improves prediction accuracy. This formulation is designed to maximize the relevance of selected features while minimizing redundancies and irrelevant features. The detailed process of optimizing QUBO for feature selection is outlined below:

$$\text{Minimize} \quad F(x) = x^T F x = \sum_{i=1}^{N} \sum_{j=i+1}^{N} F_{ij} x_i x_j \qquad (8)$$

where x is a vector of binary variables x_i (or x_j), each taking value of either 0 or 1, and F is a specified real-valued upper triangular matrix $F \in \mathbb{R}^{NxN}$ with elements F_{ij} representing weights.

2) Hyperparameter Optimization

Hyperparameter optimization (HPO) aims to find the best set of hyperparameters that maximize a model's performance. Unlike model parameters, which are learned during training, hyperparameters are set before the training process begins and govern the overall behavior of the model [20]. HPO is essential for implementing advanced ML techniques, including hybrid quantum-classical algorithms, which depend on well-optimized hyperparameters to outperform classical methods. The integration of quantum methods in hyperparameter optimization has shown significant potential in enhancing efficiency and performance [20], [21]. In the proposed model shown in Fig. 2, HPO can be enhanced using quantum-based methods like QA. The initial step involves formulating the problem as QUBO. The QUBO matrix P is an NxN matrix where each element P_{ij} represents the weight or interaction between the i-th and j-th binary variables. The formulation can be used to optimize parameters such as the learning rate and the number of layers. The matrix P is structured as follows:

$$P = \begin{bmatrix} P_{11} & P_{12} & \cdots & P_{1N} \\ P_{21} & P_{22} & \cdots & P_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ P_{N1} & P_{N2} & \cdots & P_{NN} \end{bmatrix} \qquad x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_N \end{bmatrix}$$

in this matrix, the diagonal elements P_{ii} represent the self-contributions of the binary variables, while the off-diagonal elements P_{ij} denote the interaction between different binary variables. The goal is to minimize the quadratic objective function $P(x) = x^T P_x$, where x is the vector of binary variables. This optimization identifies the best combination of hyperparameters for the machine learning prediction model. The next step is to solve the QUBO problem using quantum annealing machines, which explore the solution space to find the optimal set of hyperparameters, as outlined in the workflow in Fig. 1.

One of the primary functions of hyperparameters is to balance a model's complexity and generalization. Well-tuned hyperparameters help prevent overfitting—where the model excels on training data but fails on unseen data—and underfitting—where the model is too simplistic to capture underlying patterns. Achieving this balance is crucial for the model's real-world performance, including in predicting carbon neutrality.

3) Scenario Setting

To measure the achievement of carbon neutrality, it is necessary to create a set of scenarios to explore future carbon emissions. These scenarios are typically constructed manually by analyzing various determining factors such as GDPPC, UR, secondary industry (SI), and TEC [4], [5], [7]. This process can be optimized using QA to identify the best scenarios for achieving carbon neutrality. An example of scenario construction can be modeled as shown in Table 1 below:

TABLE I. LIST OF SAMPLE SCENARIOS

Scenario	F_1	F_2	…	F_n
S_1	Low	Medium	…	High
S_2	Medium	Low	…	High
⋮	⋮	⋮	⋮	⋮
S_n	High	High	…	Low

with S representing scenarios, F representing factors such as GDPPC, UR, and SI, and Low-Medium-High representing the set of assumptions about future development. The QUBO formulation is defined for each S dan F, where x_{ij} could represent the setting of F_1 in S_1. The optimization goal is to minimize the objective function $S(x) = \sum s_{ij} x_{ij}$, where s_{ij} are weights for each senario-factor pair. Similar to other QA optimization processes, this QUBO formulation is then processed in a quantum annealing machine as can be seen in Fig. 1 to determine the most optimal carbon neutrality scenario.

V. Conclusion

This paper presents a quantum-based prediction model for carbon neutrality by integrating machine learning (ML) and quantum annealing (QA). The model comprises of three main phases: feature selection, model development, and carbon neutrality projection. The proposed enhancements utilize QA in each phase, which previously relied on classical methods for processes such as dimensionality reduction, hyperparameter optimization, and scenario setting. QA is employed to solve combinatorial problems by converting them into QUBO format, which is then processed using quantum annealing machines to find the most optimal solutions. This study provides valuable insights into the development of prediction models that integrate ML and QA to forecast future carbon neutrality achievements. In future research, the carbon neutrality prediction framework will be implemented in real-world scenarios. Adjustments will be made to the dataset, features, and ML methods to address specific challenges. Performance measurements, such as accuracy, efficiency, and computational cost, between classical and quantum methods will also be conducted to validate the proposed approach. This continuation aims to refine the model developed in this paper for practical applications.

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