QISAP: A Machine Learning Framework for Compiler Recommendation and Quantum Circuit Analytics

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***Abstract*—The rapid evolution of quantum computing has brought forth increasingly complex quantum algorithms and hardware architectures. As quantum circuits scale in size and sophistication, the task of compiling these high-level algorithmic descriptions into efficient, hardware-executable instructions has become a critical bottleneck. This paper introduces the Quantum Integrated System Analytics Platform (QISAP), a comprehensive, open-source framework designed to provide deep insights into the structural properties of quantum circuits and to offer data-driven recommendations for compiler selection. QISAP extracts a rich set of structural and information-theoretic metrics from quantum circuits and employs a sophisticated machine learning pipeline that includes unsupervised clustering, supervised regression, and classification models. The platform achieves an R2 score of approximately 0.95 for predicting compiler performance and provides practical compiler recommendations with confidence scores. QISAP represents a significant step towards intelligent, data-driven quantum circuit compilation and optimization.**

***Index Terms*—Quantum computing, quantum circuit compilation, machine learning, compiler recommendation, quantum circuit analytics, quantum machine learning, OpenQASM, quantum optimization**

I. Overview

A. The Compilation Challenge of Quantum Circuits

Hardware architectures and quantum algorithms have become more complex as a result of the quick development of quantum computing. The process of translating these high-level algorithmic descriptions into effective, hardware-executable instructions has grown increasingly difficult as quantum circuits get bigger and more complex. Compilation is more than just translation [1], [2]; it's a complicated optimization problem with a large search space of possible gate decompositions, qubit mappings, and scheduling techniques. The decisions made during compilation have a significant impact on a quantum circuit's performance on a particular hardware backend. These decisions can alter important metrics like circuit depth, gate count, and fidelity. Qubit connectivity, gate error rates, and the non-trivial cost of two-qubit operations are just a few examples of the special limitations and opportunities that quantum systems present that make traditional compiler optimization techniques, which are typically created for classical architectures, insufficient [3], [4]. Developing a one-size-fits-all compilation strategy is made more difficult by the variety of quantum hardware platforms, each of which has its own native gate set, topology, and error characteristics. Intelligent, data-driven methods that can traverse this complicated terrain and offer optimized compilation recommendations catered to particular circuits and hardware targets are therefore desperately needed.

B. Machine Learning's Function in Quantum Computing

In many scientific and engineering fields, machine learning (ML) has become a potent paradigm for handling challenging optimization and prediction issues. Quantum computing is no different. Quantum machine learning (QML), the application of machine learning (ML) techniques to quantum circuit analysis and compilation, presents a promising path toward overcoming the drawbacks of conventional approaches [5], [6]. Using information from previously assembled circuits, ML models can be trained to forecast how well various compilation techniques will perform without requiring time-consuming, computationally costly simulations or hardware runs. This predictive capability can be used to guide the search for the best compiler configurations, greatly cutting down on the time and materials needed for circuit optimization.

Additionally, machine learning models can reveal hidden patterns and structural characteristics of quantum circuits that are not readily visible using conventional metrics, such as gate depth or count. These discoveries may result in the creation of increasingly complex optimization techniques and a better comprehension of the connection between circuit structure and performance. A fundamental change from rule-based optimization to a more flexible, data-driven approach is represented by the incorporation of machine learning (ML) into quantum compilation processes, making it possible to create quantum software stacks that are more reliable and effective.

C. QISAP: A Quantum Integrated System Analytics Overview

Given the increasing demand for intelligent compilation and analysis of quantum circuits tools, we present the Quantum Integrated System Analytics Platform (QISAP). QISAP is

a thorough, open-source framework made to offer profound understanding of the structural characteristics of quantum circuits and to provide data-based suggestions for choosing a compiler. Quantum circuits described in the OpenQASM format, a commonly used standard for quantum program representation, are ingested by the platform. From these circuits, QISAP extracts a wealth of information-theoretic and structural metrics, comprising the number of qubits, circuit depth, gate counts, gate densities, and a new metric known as entropy of instruction. These measurements form the basis of an advanced machine learning pipeline that comprises supervised regression, unsupervised clustering, and models for classification. The unsupervised learning component gives a high-level overview of the dataset by clustering circuits into structurally similar groups. After being trained on a sizable corpus of compiled circuits, supervised models are able to forecast important performance metrics and suggest the best compiler for a particular circuit. Researchers and practitioners can use the entire platform thanks to its interactive web-based dashboard and automated PDF report generation system. The goal of QISAP is to close the gap between designing quantum circuits and effective implementation by offering a strong, intuitive tool for analysis, optimization, and instruction.

D. Principal Inputs of the Paper

The QISAP is thoroughly described and analyzed technically in this paper, emphasizing its innovative contributions to the study and compilation of quantum circuits. This work makes three major contributions. First, we present an extensive collection of metrics, such as the new instruction_entropy metric, for describing the information-theoretic and structural characteristics of quantum circuits, which measures how different gates are used in a circuit. We offer a mathematical analysis of this metric and talk about how it relates to comprehending circuit complexity. Second, we offer a strong machine learning pipeline that makes use of these metrics to predict compiler performance with high accuracy. The strong correlation between circuit structure and compilation results is demonstrated by our regression models, which predict a proxy for compiler performance with an R2 score of roughly 0.95. Third, we create a useful and intuitive compiler recommendation system that offers not just a suggested compiler but a complete probability distribution across all available compilers, as well as a confidence score. Based on the model's predictions, this system enables users to make well-informed decisions. Along with discussing the shortcomings of the current implementation and potential avenues for further research, the paper compares QISAP with other tools and frameworks that are currently in use, such as Qiskit Machine Learning.

II. The Architecture and Core Components of the QISAP Platform

A. Data Flow and System Architecture

The modular architecture of the QISAP platform allows for a clear separation of responsibilities and permits an adaptable, expandable workflow. Each of the system's many essential parts is in charge of a particular phase of the analysis and recommendation process. Quantum circuits in the OpenQASM format are ingested to start the data flow. A metric extraction pipeline then parses and processes these circuits, calculating an extensive set of features for every circuit. The resulting metrics serve as the foundation for the ensuing machine learning analysis and are saved in an organized manner. Data preprocessing, model training, and prediction are some of the steps in the machine learning pipeline, which is the platform's central component. The compiler recommendation system, which gives users personalized advice, is then powered by the trained models. Lastly, the platform provides a number of interfaces for working with the analysis's findings, such as an automated PDF report generator, an interactive web dashboard, and a command-line tool. From command-line enthusiasts to researchers who prefer a graphical interface, this multifaceted approach guarantees that the insights produced by QISAP are accessible to a broad range of users.

1) Quantum Circuit Ingestion and Parsing: The QISAP workflow's first step entails ingesting and parsing quantum circuits. Circuits described in the OpenQASM 2.0 format, a commonly used standard for representing quantum programs, can be accepted by the platform. This task is handled by the parse_circuits.py script [7], [8], which makes use of the Qiskit and Cirq libraries to load the circuit files. IBM created Qiskit, a complete open-source SDK for quantum computing that offers resources for building, modeling, and operating quantum circuits. Another potent framework for creating, modeling, and executing quantum circuits on Google's quantum processors is Cirq, which was created by the company. QISAP guarantees broad compatibility with a variety of quantum programming tools and ecosystems by supporting both of these well-known frameworks. The process of parsing entails reading the .qasm file, building an internal circuit representation, and checking the syntax and semantics of the circuit. This action is essential to guaranteeing that the subsequent metric extraction and analysis are carried out on an accurate and precisely defined circuit design. The platform's ability to process circuit files in batches enables the analysis of sizable datasets, which is crucial for building strong machine learning models.

2) The Extraction of Metrics Pipeline: A quantum circuit is sent to the metric extraction pipeline after it has been successfully parsed. The extract_metrics.py script implements this pipeline. This pipeline is in charge of calculating an extensive collection of features that describe the circuit's information-theoretic and structural characteristics. The extracted metrics are intended to capture different facets of the structure and complexity of the circuit, offering a rich feature set for the models used in machine learning. Nine core metrics are calculated for every circuit, which are subsequently saved for later examination in a CSV file. Among these metrics are fundamental structural characteristics like the number of qubits (num_qubits), the counts of various gate types (cx_count, 1q_count, 2q_count, and total_ops) as well as the circuit depth (depth). The pipeline calculates a number of derived metrics in addition to these common ones, which offer more in-depth

understanding of the circuit's structure. Among these is the gate_density, which calculates the proportion of all gates to the product of depth and qubits, and the 2q_1q_ratio, which measures the balance between two-qubit and single-qubit operations. Additionally, the pipeline presents instruction_entropy, a new information-theoretic metric that quantifies the Shannon entropy of the gate usage distribution and thus provides a measure of the circuit's operational diversity [9], [10]. Lastly, a compiler_score is calculated to represent a particular compiler's performance on the circuit, acting as the regression models' target variable.

3) The Learning Machine Pipeline: The core component of the QISAP platform is the machine learning pipeline, which is in charge of developing the models that underpin its recommendation and prediction systems. The pipeline is implemented in two primary scripts: ml_pipeline.py and ml_extended_models.py. The ml_pipeline.py script manages the preliminary training of the fundamental models, such as an unsupervised circuit K-Means clustering model for grouping and a Random Forest Regressor to forecast the compiler_score. The script starts by loading the compiled metrics from the extraction pipeline's CSV file. After that, it carries out any required data preprocessing, including addressing missing values or feature scaling. The circuits are grouped by training the K-Means model into a predetermined number of clusters (k=4) according to how similar their structures are. This grouping gives a high-level summary of the data and can be used to find unique circuit classes. After that, the Random Forest Regressor is trained to forecast the compiler_score according to the metrics that were extracted. This pipeline is expanded by the ml_extended_models.py script, which trains extra regression models to forecast additional circuit characteristics, like the depth and instruction_entropy. This method of multi-target regression enables the platform to offer a more thorough examination of the circuit's properties. Because trained models are stored on disk as .joblib files, they are easily accessible for the platform's recommendation system and other elements.

4) Reporting and Visualization Suite: In order to facilitate the accessibility and interpretation of the analysis results, QISAP incorporates a full suite of reporting and visualization tools. This collection includes multiple Python scripts that produce a range of charts and plots to highlight the main conclusions of the examination. Basic distribution plots are produced by the visualize_metrics.py script, including histograms for every metric that was extracted, giving a brief summary of the dataset's qualities. Additionally, it creates pairplots to show the connections between pairs of characteristics, assisting in the discovery of patterns and correlations. More complex visualizations pertaining to the cluster analysis are produced by the visualize_research_graphs.py script. The circuits embedded in the principal component analysis (PCA) space are shown in a 2D scatterplot, where each point is colored according to its cluster label. The clustering results and the general structure of the dataset are visually represented in this plot in an understandable manner. Additionally, the script creates radar charts for every cluster, showing the average values of important metrics for circuits in that cluster, including the 2Q/1Q ratio, instruction entropy, and gate density. These radar charts provide a succinct overview of each cluster's unique features. Lastly, the generate_pdf_reports.py script creates detailed PDF reports automatically for specific circuits. These reports offer a thorough and easily shareable record of the analysis by including an overview of the circuit's metrics, the predictions made by the ML models, and the pertinent visualizations.

B. Fundamental Measures for Circuit Description

The QISAP platform's efficacy depends on its capacity to extract significant and predictive characteristics of quantum circuits. In order to achieve this, the platform calculates a wide range of metrics that represent different facets of circuit complexity and structure. These metrics fall into three general categories: information-theoretic metrics, derived metrics, and structural metrics. Machine learning models can learn the intricate relationships between circuit properties and compiler performance thanks to this multifaceted approach to circuit characterization, which guarantees that they have access to a rich and instructive feature set. The goal behind choosing these metrics was to record not just the circuit's fundamental characteristics, like its size and depth, as well as more subtle traits that are indicative of the type of quantum quantum computation being carried out. QISAP offers a comprehensive picture of the circuit by integrating these various metrics, which is necessary for precise performance prediction and optimization.

1) Structural Metrics: Gate Counts, Depth, and Qubit Counts: The most basic metrics that QISAP extracts are the structural metrics, which give a basic description of the size and complexity of the circuit. These metrics form the basis for more complex characterizations and are crucial for any analysis of quantum circuits. One of the main factors influencing the hardware resources required is the number of qubits needed to complete the circuit, which is simply counted by the num_qubits metric. The length of the circuit's longest path from any input to any output is measured by the depth metric, which also indicates how many time steps are needed to run the circuit serially. In general, a lower depth is preferred because it suggests a quicker execution time and a decreased vulnerability to decoherence. Moreover, the platform counts the number of gates of various kinds, such as the cx_count (the number of CNOT gates, a common two-qubit entangling gate), the 1q_count (the number of single-qubit gates), and the 2q_count (the total number of two-qubit gates). These gate counts offer a more thorough perspective of the circuit's makeup and are frequently associated with the computation's overall fidelity, since two-qubit gates generally exhibit higher error rates than single-qubit gates. Lastly, a basic indicator of the circuit's overall size, the total_ops metric gives a straightforward count of all the gates in the circuit.

2) Derived Metrics: 2-Qubit to 1-Qubit Ratio and Gate Density: Apart from the fundamental structural metrics, QISAP calculates a number of derived metrics that give

more detailed information about the efficiency and structure of the circuit. These metrics are intended to capture more subtle characteristics of the circuit and are computed from the primary metrics. The ratio of the total number of gates (total_ops) to the product of the circuit depth and the number of qubits (depth * num_qubits) is known as the gate_density metric. The circuit's gate density is indicated by this metric. A circuit that is highly parallelized and carrying out many operations at once may be indicated by a high gate density, whereas a more serialized computation with a large amount of idle time for certain qubits may be suggested by a low gate density. The ratio of two-qubit gates (2q_count) to single-qubit gates (1q_count) is known as the 2q_1q_ratio metric. In the context of near-term quantum devices, where two-qubit gates are frequently the main source of error, this metric is especially crucial. Due to its heavy reliance on the noisier two-qubit operations, a circuit with a high 2q_1q_ratio may be more difficult to implement faithfully on existing hardware. The machine learning models can develop a more complex comprehension of the circuit's structure and its possible performance across various hardware systems by taking into account these derived metrics.

3) Information-Theoretic Metrics: Instruction Entropy: Among the QISAP platform's innovative features is the launch of an information-theoretic metric called instruction_entropy. In order to measure the complexity of the instruction set needed to implement the algorithm, this metric is intended to quantify the diversity of gate usage within a quantum circuit. The instruction entropy is calculated using the Shannon entropy formula, a basic idea in the field of information theory [9]. It gives an indication of how unpredictable or random the circuit's gate sequence is. An elevated instruction entropy signifies a circuit with a varied and erratic gate sequence, whereas a circuit with a low entropy has a gate sequence that is more regular and structured. Circuits that are likely to be difficult for compilers to optimize and circuits that might be more prone to specific kinds of errors can both be found using this metric. Understanding the characteristics of quantum circuits and forecasting how well they will function on actual quantum devices require a comprehensive and multifaceted characterization, which is provided by the combination of these three types of metrics.

4) Shannon Entropy of Gate Usage: A Mathematical Formulation: The instruction_entropy metric in QISAP is a direct application of the classical Shannon entropy formula to the distribution of gate types in a quantum circuit. Let a quantum circuit C consist of a set of N unique gate instructions $\{g_1, g_2, \ldots, g_N\}$.

Let us assume that for every gate type g_i, we let p_i be the probability of its occurrence in the circuit, which is calculated as the number of times g_i appears divided by the total number of gates. The instruction entropy, H_{inst}, will then be defined as:

$$H_{\text{inst}}(C) = -\sum_{i=1}^{N} p_i \log_2(p_i)$$

The uncertainty or information content related to the gate distribution is measured by this formulation. Since there is no uncertainty, a circuit with just one kind of gate, for example, only CNOT gates will have an entropy of 0. The maximum entropy that can exist in a circuit with a perfectly uniform distribution of gate types is $\log_2(N)$.

The structural diversity of a circuit's implementation can be effectively captured by this metric. A circuit designed for a particular hardware platform, for instance, may have low entropy since it only makes use of the platform's native gate set. On the other hand, a circuit that is more abstract or high-level may have a higher entropy, which would indicate a wider variety of logical operations. The QISAP platform uses this metric as a key feature for its machine learning models, which have shown that it is a significant predictor of compiler performance, alongside other structural metrics like gate counts and depth [9].

C. The Reporting and Interactive Dashboard System

The platform features an automated reporting system and an intuitive interactive dashboard to make QISAP's potent analytical capabilities available to a wide audience. These elements offer user-friendly graphical user interfaces for examining the analysis findings, facilitating users' understanding of the characteristics of their quantum circuits and the machine learning models' suggestions. Streamlit, a well-known open-source framework for developing data applications, is used to build the dashboard, and the reporting system produces comprehensive PDF documents for every examined circuit. When combined, these resources offer a thorough and adaptable method of interacting with the QISAP platform, meeting the requirements of both novice and seasoned researchers.

1) Circuit Analysis in Real Time and Visualization: The interactive web dashboard is the focal point of the QISAP user interface, started with the command streamlit run streamlit_dashboard.py. This dashboard offers an interactive, real-time setting for quantum circuit analysis and visualization. Among the dashboard's primary functions is a circuit selector that permits users to select a particular circuit for in-depth examination from the dataset. The dashboard presents the circuit's primary metrics in an easy-to-understand manner after it has been chosen. Additionally, the dashboard has a number of interactive visualizations, including a PCA cluster map, which illustrates the chosen circuit's location within the dataset's overall landscape, and a radar chart that shows the distinctive characteristics of the cluster the circuit is a part of. Based on the user's choices, these visualizations are updated dynamically, offering an interesting and educational method to examine the data. A raw data table is another feature of the dashboard that lets users examine the underlying metrics for each circuit in the dataset. The dashboard is an effective tool for exploratory data analysis and for developing a deeper comprehension of the connections between circuit structure and performance because of its interactive visualizations and direct data access.

2) Automated PDF Report Generation: The generate_pdf_reports.py script implements QISAP's automated PDF report generation system, which is in addition to the interactive dashboard. The purpose of this system is to generate a comprehensive, independent report for every circuit in the dataset, offering a thorough synopsis of the findings of the analysis. A summary of the circuit's primary metrics, the predictions made by the machine learning models, and numerous visualizations are just a few of the many details included in the automatically generated reports. The report's visualizations include a PCA map that displays the circuit's location within the entire dataset and a radar chart that displays the characteristics of the cluster to which the circuit belongs. A thorough analysis of the model's predictions, along with the suggested compiler and related confidence score, is also included in the reports. These PDF reports are a great way to record the findings of the analysis, share them with colleagues, and use them as teaching tools. They supplement the interactive dashboard's real-time, exploratory nature by offering a permanent and easily accessible record of the analysis.

III. The Machine Learning Pipeline: Predictive Models and Analysis

The QISAP platform's primary analytical engine, the machine learning pipeline, is in charge of converting the raw circuit metrics into useful insights and suggestions. A multifaceted view of the data is provided by the pipeline's comprehensive design, which combines supervised and unsupervised learning techniques. Circuits are naturally grouped according to their structural characteristics using the unsupervised learning component, which is based on K-Means clustering. This helps to distinguish different circuit classes and offers a high-level overview of the dataset. Regression and classification models are part of the supervised learning component, which is used to forecast certain results, like compiler performance, and to provide suggestions. Whereas the classification model is trained to predict discrete labels, like the suggested compiler, the regression models are trained to predict continuous values, like the compiler_score. The scikit-learn library, a robust and popular Python machine learning library that offers a comprehensive set of tools for model training, evaluation, and deployment, serves as the foundation for the entire pipeline.

A. Unsupervised Learning: Circuit Clustering

Using unsupervised learning techniques on the circuit metrics dataset is the initial stage of the QISAP machine learning pipeline. Finding hidden patterns and structures in the data without any prior knowledge of the anticipated results is the aim of this step. Clustering algorithms are used to accomplish this, grouping comparable data points according to a predetermined distance metric. We can obtain a high-level understanding of the different circuit types in our dataset and their relationships by grouping the circuits according to their structural characteristics. The supervised learning tasks that follow can be guided by this information, which also offers important insights into the nature of quantum circuit design.

1) Structural K-Means Clustering: K-Means clustering is the main unsupervised learning method used in QISAP. The K-Means algorithm is a straightforward but effective technique for dividing a dataset into a fixed number of clusters (k). Each data point is iteratively assigned to the cluster with the closest centroid (the cluster mean) by the algorithm, which then updates the centroids in light of the new assignments. The quantum circuits are the data points in the context of QISAP, and the extracted metrics (such as num_qubits, depth, cx_count, etc.) are the features. The algorithm is designed to produce k=4 clusters, a decision made after the dataset was empirically analyzed. The clusters that are produced are collections of circuits that share structural similarities. Circuits with a high gate density and a large number of qubits, for instance, might be found in one cluster, whereas circuits with a low gate density and a small number of qubits might be found in another. The dataset is usefully summarized by this clustering, which can also be used to find different classes of circuits that may need distinct compilation techniques.

2) Cluster Visualization using PCA and Radar Charts: In order to facilitate the interpretation of the clustering analysis results, QISAP incorporates a collection of visualization tools that offer clear depictions of the clusters. Principal Component Analysis (PCA), a dimensionality reduction technique that can be used to project high-dimensional data onto a lower-dimensional space, is one of the primary visualization techniques employed. The circuit metrics in QISAP constitute a high-dimensional feature space. We can see the clusters and their connections by projecting the circuits onto a 2D plane using PCA. The resulting scatterplot offers a concise and understandable summary of the clustering results, with points colored according to their cluster label. QISAP summarizes each cluster's characteristics using radar charts in addition to the PCA plot. A radar chart is a two-dimensional graphical representation of multivariate data that shows three or more quantitative variables on axes that all start at the same point.

B. Supervised Education: Regression and Classification

The QISAP machine learning pipeline's supervised learning component is in charge of teaching models to forecast particular results using the circuit metrics that have been extracted. This includes regression models that forecast continuous values as well as classification models that forecast distinct labels. Key performance metrics, like the compiler_score, are predicted by the regression models, while recommendations, such as the best compiler for a particular circuit, are made using classification models. The scikit-learn framework serves as the foundation for the entire supervised learning pipeline, which offers an extensive collection of resources for training, assessing, and deploying models.

1) Random Forest Regressor for Performance Prediction: The Random Forest Regressor is the main regression model utilized in QISAP. This model is an ensemble learning technique that generates a more reliable and accurate result by combining the predictions of several decision trees. Because it can capture intricate, non-linear relationships between the

circuit metrics and the target variable, the Random Forest Regressor is ideally suited to the task of predicting compiler performance [11], [12]. The model learns to predict the score for new, unseen circuits based on their structural properties after being trained on a dataset of circuits with known compiler_score values. One important input for the recommendation system is the expected performance of a given compiler on a given circuit, which QISAP can quantitatively evaluate through the use of a Random Forest Regressor.

2) Random Forest Classifier for Compiler Recommendation: To recommend compilers, QISAP employs a Random Forest Classifier in addition to the regression model. The best compiler for a specific circuit from a list of preset choices is predicted by this model. In order to determine which structural characteristics are most indicative of a successful match between a circuit and a compiler, the classifier is trained on a dataset of circuits with known optimal compilers. The most likely candidate can be chosen using the classifier's output, which is a probability distribution over the available compilers. Using a Random Forest Classifier [13], [14], users can save a great deal of time and effort during the compilation process by enabling QISAP to offer a data-driven recommendation for the best compiler to use for a particular circuit.

C. Model Assessment and Feature Relevance

One crucial phase in the QISAP pipeline is the assessment of the machine learning models because it gives an indication of how predictive the models are and aids in determining which features are most crucial for forecasting. Numerous metrics are used in the evaluation, such as accuracy for the classification models and R2 scores for the regression models. The Random Forest models' built-in feature of feature importance analysis offers important information about the variables that most predict compiler performance.

1) Predictive Power: R2 Values and Precision: Standard metrics for regression and classification tasks are used to assess the QISAP machine learning models' predictive ability. The compiler_score is predicted by the Random Forest Regressor, which obtains a high R2 score of roughly 0.95, meaning that 95% of the variance in the target variable can be explained by the model. This is a powerful finding that indicates the features that were extracted are closely related to the performance of the compiler. The accuracy of the Random Forest Classifier for predicting the best compiler is roughly 0.92, which indicates that 92% of the time, the model correctly determines the best compiler. These high scores show how well the QISAP machine learning pipeline works and give the platform's recommendation system a solid base.

2) Important Compiler Predictive Features: The Random Forest models' feature importance analysis offers useful information about the variables that most accurately predict compiler performance [14], [15]. The evaluation indicates that the most crucial characteristics for estimating the compiler_score are the depth, cx_count, total_ops, 1q_count, and 2q_count. Given that these metrics are known to have a strong correlation with quantum circuit performance on NISQ hardware. The significance of the metrics 2q_count and cx_count are especially significant because two-qubit gates are frequently the main cause of error in modern quantum devices. The reality that these characteristics are found to be the most significant predictors offers a solid confirmation of the QISAP feature extraction pipeline and contributes to the development of trust in the platform's suggestions.

IV. The Compiler's Suggestion System

A. The Engine for Suggestions: enhanced_circuit_recommender.py

The QISAP machine learning pipeline's practical use is the compiler recommendation system, giving users practical guidance on the best compiler to use for a given quantum circuit. The enhanced_circuit_recommender.py command-line tool, which implements the system, receives a set of circuit metrics as input and returns a full probability distribution over the available compilers, a recommended compiler, and a confidence score. This enables users to view more than just the top suggestion, but also to comprehend the uncertainty of the model and to take into account alternate choices in the event that confidence is low. The engine that makes recommendations is driven by the trained Random Forest Classifier, which has learned to determine which circuit structural characteristics are most indicative of a good match with a specific compiler.

B. Input and Output Details

A collection of circuit metrics is fed into the enhanced_circuit_recommender.py script, which can be read from a file or supplied as command-line arguments. The extract_metrics.py script extracts the same metrics that are needed, including num_qubits, depth, cx_count, 1q_count, 2q_count, total_ops, gate_density, 2q_1q_ratio, and instruction_entropy. The script's output is a thorough report that comprises the full probability distribution across all available compilers, the suggested compiler, and the recommendation's confidence score. This thorough output gives users all the data they require in order to make an informed choice regarding the appropriate compiler to use.

C. Confidence Scores and Probability Distributions

The QISAP recommendation system's provision of confidence scores and probability distributions is one of its primary features. The model's level of certainty in its recommendation is gauged by the confidence score, which is determined using the predicted probabilities of the Random Forest Classifier. When the model's confidence score is high, it means that it is highly certain of its recommendation; when it is low, it means that the circuit is unclear, and multiple compilers might be equally appropriate. The complete probability distribution provides a more detailed view of the model's predictions, displaying the expected likelihood for every compiler that is available. This enables users to view the relative likelihood of the other options in addition to the top recommendation. This data can be especially helpful when the top recommendation has a low confidence score because it lets users think about the next-best options.

V. Mathematical Analysis of Circuit Representation and Entropy

A fundamental component of the QISAP platform is the quantitative characterization of quantum circuits, which makes it possible to use machine learning methods for compiler recommendation and performance prediction. A crucial component of this characterization is the measurement of the complexity or information content of a circuit's structure. The instruction_entropy metric used by QISAP is based on the gate usage frequencies' classical Shannon entropy. Although this offers a useful and computationally effective measure of circuit diversity, it is essentially a classical abstraction of a quantum system. This section offers a thorough mathematical analysis of this metric, compares it to von Neumann entropy, the fundamental quantum information measure, and investigates a more sophisticated, quantum-aware alternative known as pseudo-entropy. The purpose of this analysis is to place QISAP's present capabilities in the larger context of quantum information theory and to identify areas where its analytical framework can be improved in the future.

A. Classical Representation of Quantum Circuits

It is crucial to establish the mathematical frameworks used to represent quantum circuits classically before exploring entropy measures. These representations are the substrate upon which metrics like instruction_entropy are calculated and are fundamental to the entire QISAP pipeline. Despite being quantum, quantum circuits are described and controlled by means of classical data structures, mainly directed acyclic graphs (DAGs) and gate matrices. These abstractions enable analysis and simulation by capturing the crucial details regarding the order and kind of operations performed on qubits on traditional computers. The kinds of analyses that can be carried out and their computational complexity are greatly influenced by the representation that is chosen. For example, although gate matrices offer a comprehensive explanation of the unitary evolution of the quantum state, they suffer from exponential scaling with the number of qubits. However, DAGs provide a more scalable depiction of the circuit's structure by emphasizing the dependencies among gates rather than their exact unitary action. As a result, they are ideal for the type of structural analysis carried out by QISAP.

1) Gate Matrices and Tensor Products: A quantum circuit is essentially a series of quantum gates, each of which operates on one or more qubits as a unitary operation. Each gate can be represented mathematically by a unitary matrix. A two-qubit gate is a 4×4 unitary matrix, whereas a single-qubit gate is a 2×2 unitary matrix. The tensor product of a gate's matrix with identity matrices for the qubits it does not act on describes the gate's action on a particular set of qubits inside a larger circuit. As an illustration, if a two-qubit gate U affects a three-qubit system's qubits 1 and 3, its overall effect is symbolized by the matrix $I \otimes U \otimes I$, in which I is the 2×2 identity matrix. The matrices that represent each gate in the sequence are then multiplied to determine the total unitary transformation of the entire circuit. This representation of a matrix offers a thorough and clear explanation of how the circuit affects any input quantum state. Nevertheless, the overall circuit matrix's size increases exponentially with the quantity of qubits ($2^n \times 2^n$ for an n-qubit circuit), rendering all but the smallest circuits computationally unfeasible. The main driving force behind the use of more abstract representations, such as DAGs, in useful analysis tools is this exponential scaling.

2) Directed Acyclic Graphs (DAGs) for Circuit Structure: Directed Acyclic Graphs (DAGs) are frequently used to depict quantum circuits in order to get around the computational constraints of full matrix representation. Each graph node in this model represents a quantum gate, and the directed edges show how qubits move between gates. An essential prerequisite for a legitimate quantum circuit in which operations are applied successively in time is the absence of loops, which is guaranteed by the "acyclic" property. The structural characteristics of a circuit, including its depth (the longest path from an input to an output), the number of gates, and the dependencies between operations, can be captured with great efficiency using this representation. By using this DAG representation as the direct input for its Graph Neural Network (GNN) model, the MQT Predictor, a related hardware selection tool, eliminates the need for manual feature extraction. With this method, all of the information encoded in the graph is preserved and the model is able to learn directly from the circuit's structure. In contrast, QISAP extracts a set of metrics or summary statistics from the DAG representation as a step in between. These metrics are then utilized as features for its machine learning models. One of the main differences between various methods of quantum circuit analysis is the trade-off between employing condensed features (metrics) and maintaining full structural information (DAGs).

B. Examination of the instruction_entropy metric

One of the main features of QISAP is the instruction_entropy metric, which measures the variety and distribution of gate types in a quantum circuit. It is computed as the frequency-specific Shannon entropy of each distinct gate instruction in the circuit. This yields a single, scalar value that encapsulates the "richness" of the instruction set of the circuit. A circuit that heavily relies on a small number of gate types will have a low instruction entropy, whereas a circuit that uses a wide variety of gate types at roughly equal frequency will have a high instruction entropy. This metric is a sensible option for extensive analysis because it is easy to understand and computationally efficient to compute. The quantum characteristics of the gates themselves, such as their capacity to produce entanglement or their particular unitary action, are not captured by its classical nature. This section gives the metric a formal definition, contrasts it with the quantum-native von Neumann entropy, and presents a more advanced substitute, pseudo-entropy, which connects quantum mechanics and classical information theory.

1) Shannon Entropy of Gate Usage: A Mathematical Formulation: QISAP's instruction_entropy metric is a straightforward implementation of the traditional Shannon entropy

formula applied to the distribution of gate types in a quantum circuit. Allow a quantum circuit C to consist of a set of N distinct gate instructions $\{g_1, g_2, \ldots, g_N\}$. For each gate type g_i, let p_i be the likelihood that it will occur in the circuit, determined as the number of times g_i appears divided by the total number of gates. The instruction entropy, H_{inst}, is then defined as:

$$H_{\text{inst}}(C) = -\sum_{i=1}^{N} p_i \log_2(p_i)$$

This formula calculates the degree of uncertainty or information content connected to the distribution of gates. A circuit with a single kind of gate (for example, only CNOT gates) will have an entropy of 0, since there is no uncertainty. A circuit with a flawlessly consistent distribution of gate types will have the maximum possible entropy, which is $\log_2(N)$. The structural diversity of a circuit's implementation can be effectively captured by this metric. A circuit designed for a particular hardware platform, for instance, may have low entropy since it only makes use of the platform's native gate set. On the other hand, a circuit that is higher level or more abstract may have a high entropy, representing a wider range of logical processes. This metric is a crucial component of the QISAP platform's machine learning models, which have demonstrated that it is a key indicator of compiler performance, along with other structural parameters like depth and gate counts.

2) Comparison with Quantum Entropy Measures (Von Neumann Entropy): Shannon entropy is a strong and useful tool in classical information theory. However, when we try to apply it to quantum systems—for example, in the case of the instruction_entropy metric—it becomes only an abstraction that does not fully capture the quantum nature of information.

In quantum mechanics, the main measure of information is the von Neumann entropy. For a quantum system that is described by a density matrix ρ, the von Neumann entropy is defined as [16]:

$$S(\rho) = -\text{Tr}(\rho \log_2 \rho)$$

This formula is considered the quantum version of Shannon entropy. The key difference is that instead of working on a classical probability distribution, it works directly on the quantum state itself, which is represented by the density matrix ρ.

The von Neumann entropy tells us how uncertain or "mixed" a quantum state is. A pure state, which has a well-defined state vector, has zero von Neumann entropy. On the other hand, a maximally mixed state—which is a statistical mixture of all possible basis states with equal probability—has the highest entropy.

Now, comparing this to the instruction_entropy metric: instruction_entropy is more like a traditional way of counting or measuring how diverse the operations in a circuit are. It does not directly measure how much information the state of the circuit actually contains. Importantly, it ignores the deeper quantum properties of the gates, such as their unitary actions or their ability to create entanglement.

For example, two circuits might show the same instruction_entropy but end up producing quantum states with very different von Neumann entropies, depending on which gates are chosen and how they are arranged.

This shows us a clear limitation: using classical-style metrics like instruction_entropy to describe quantum systems leaves out important quantum details. This motivates the need for new, more quantum-aware metrics that better reflect the true informational nature of quantum states.

3) Complex Quantum-Aware Measures: Pseudo-Entropy and Linear Entropy: The investigation of more complex, quantum-aware metrics is motivated by the limitations of classical Shannon entropy in describing quantum phenomena. These metrics, which provide a closer link to the underlying quantum state of a circuit, include pseudo-entropy and linear entropy. These metrics take into account the quantum characteristics of the operations themselves, such as their separation from the identity operation and their capacity to produce entanglement, in addition to the basic frequency of gate types. The incorporation of such metrics into a platform such as QISAP represents an important step toward a more thorough and predictive characterization of quantum circuits. These quantum-aware metrics may offer a richer feature set for machine learning models, which could result in more precise predictions of compiler performance and circuit behavior on actual hardware, even though they are computationally more demanding than instruction_entropy. The theoretical underpinnings of linear entropy and pseudo-entropy are examined in this section, along with their possible uses in the context of quantum circuit analysis.

a) Linear Entropy and Its Use in Quantum Circuits: Another crucial metric in quantum information theory, linear entropy is frequently employed as a more straightforward approximation of von Neumann entropy. Its definition is $S_L(\rho) = 1 - \text{Tr}(\rho^2)$, where ρ is the quantum state's density matrix. The state's purity, or $\text{Tr}(\rho^2)$, is a measure of how near it is to being a pure state, or one with zero entropy. For measuring the level of entanglement in a quantum system, linear entropy is especially helpful [17], [18]. A measure of the entanglement between two parts of a bipartite system can be obtained from the linear entropy of the reduced density matrix of one of the subsystems. This has been used to examine the dynamical characteristics of entanglement in studies of coupled qubit systems. The amount of entanglement produced by a circuit, which is a crucial component of its computational capacity and noise sensitivity, can be measured using linear entropy in the context of quantum circuits. A complex and possibly delicate quantum state is indicated by a circuit with a high linear entropy that produces a high degree of entanglement. A key component of quantum circuit performance on NISQ devices is entanglement properties, which QISAP could be able to characterize more effectively by adding linear entropy to its feature set.

b) The Linear Cross-Entropy Benchmarking (Linear XEB): The Linear Cross-Entropy Benchmarking (Linear XEB) fidelity is a related idea that has become more well-known in the field of quantum computing. Google famously used this metric to show off their Sycamore processor's quantum computational advantage [19]. The Linear XEB quantifies the degree to which a probability distribution produced by a quantum circuit or a classical simulator resembles the optimal output distribution of a random quantum circuit [20]. It is described as:

$$F_C(p) = 2^n \mathbb{E}_{x\sim p}[q_C(x)] - 1$$

where $q_C(x)$ is the optimal probability of obtaining the bitstring x from circuit C, n is the number of qubits, and p is the output distribution under test. A trivial simulator (such as the uniform distribution) is indicated by a value of 0, whereas a non-trivial correlation with the ideal output is indicated by a value greater than 0. The Linear XEB is a useful tool for comparing the performance of quantum hardware and validating the outcomes of quantum computations, even though it is not a direct measure of entropy. It offers a useful method for evaluating the output fidelity of a quantum circuit, which is a crucial component of its overall functionality. The ideas behind Linear XEB may lead to new QISAP metrics that compare a compiled circuit's output to a perfect, noiseless simulation. This would give a clear indication of how well the compiler preserved the circuit's intended functionality.

c) Pseudo-Entropy: An Extension of Von Neumann Entropy: Pseudo-entropy is a recently introduced concept that generalizes von Neumann entropy beyond density matrices to the broader class of quantum operators, such as the unitary gates that form a quantum circuit. This extension becomes especially relevant in quantum machine learning (QML), where the primary objective is to encode classical data into quantum states through parameterized quantum circuits, also called quantum feature maps.

A recent study proposes a way to compute the "expanded pseudo-entropy" [21], applying it not just to the final density operator but to each operator in the feature map. The motivation here is to evaluate how effectively a given encoding scheme transfers classical information into the quantum circuit and retains it throughout. The intuition is to think of each data point as carrying a certain "energy" that gets transferred into a quantum gate. By studying the pseudo-entropy of the operators produced, one can measure the quality of that encoding. This method is claimed to generalize other QML evaluation approaches such as expressibility and expressivity, offering a broader and more informative metric of a circuit's ability to process information.

For platforms like QISAP, integrating pseudo-entropy would enable deeper circuit analysis, especially for QML-specific designs, by introducing a metric that directly reflects the quantum properties of the gates themselves.

d) Linear Entropy and Its Use in Quantum Circuits: Linear entropy is another useful metric in quantum information theory [17], [18]. It is often used as a simpler way to approximate von Neumann entropy.

It is defined as:

$$S_L(\rho) = 1 - \text{Tr}(\rho^2)$$

Here, ρ is the density matrix of the quantum state. The part $\text{Tr}(\rho^2)$ is called the purity of the state. Purity tells us how close the state is to being "pure" (which means zero entropy).

Linear entropy is very useful for measuring entanglement in a quantum system. For example, in a system of two parts (a bipartite system), the linear entropy of one part's reduced density matrix shows how entangled the two parts are.

This has been used in studies of coupled qubits to understand how entanglement changes over time. In the context of quantum circuits, linear entropy can tell us how much entanglement a circuit creates. This is important because entanglement is linked to computational power, but also to sensitivity to noise.

A circuit with a high degree of entanglement will also have a high linear entropy, meaning it is creating a very complex and possibly fragile quantum state. If QISAP uses linear entropy, it would gain a strong tool to measure the entanglement of circuits, which is crucial for performance on today's NISQ devices.

e) The Linear Cross-Entropy Benchmarking (Linear XEB): Another related concept is Linear Cross-Entropy Benchmarking (Linear XEB) fidelity. This metric became well known when Google used it to show quantum computational advantage with their Sycamore processor [19].

Linear XEB measures how closely the output distribution of a circuit (or simulator) matches the ideal output of a random quantum circuit. It is defined as:

$$F_C(p) = 2^n \mathbb{E}_{x\sim p}[q_C(x)] - 1$$

Here, n is the number of qubits, p is the tested output distribution, and $q_C(x)$ is the ideal probability of getting the bitstring x from circuit C.

- A value of 0 means the distribution is trivial (like a uniform random guess). - A value greater than 0 means the output has some correlation with the ideal distribution.

Even though Linear XEB is not a direct entropy measure, it is very powerful for testing quantum hardware and checking if quantum computations are correct. It is a practical way to see how faithful a circuit's output is.

For QISAP, the principles of Linear XEB could inspire new metrics that compare a compiled circuit's output with an ideal, noiseless simulation. This would give a direct measure of how well the compiler preserves the circuit's intended behavior.

C. Quantum Computing Benchmarking and Evaluation Metrics

The assessment of hardware, compilers, and quantum circuits is a challenging task that calls for a multifaceted strategy. There isn't a single metric that can account for every facet of performance, and the evaluation's particular objectives greatly influence which metrics are used. The main objective

of QISAP is to predict the compiler's performance on a specific circuit, which necessitates a thorough comprehension of the variables affecting that performance. These elements can be roughly divided into three categories: application-centric metrics, which describe the computation's end result; compiler-centric metrics, which describe the characteristics of the compiled circuit; and hardware-centric metrics, which describe the characteristics of the actual device. To give a full picture of the system's performance, a thorough evaluation framework needs to take into account all three of these viewpoints. The main metrics in each of these categories are summarized in this section along with their applicability to the QISAP platform.

1) Hardware-Centric Metrics: Quantum Volume and CLOPS: These metrics are intended to describe the performance of a quantum processing unit (QPU) itself, independent of any specific application or compiler. These metrics provide a high-level summary of the device's capabilities and are often used by hardware vendors to benchmark their systems. Quantum Volume (QV), which quantifies the largest square circuit (i.e., a circuit with the same number of qubits and depth) that can be executed on a device with a fidelity above a certain threshold, is one of the most well-known hardware-centric metrics [2], [22]. QV is a comprehensive metric that provides a single figure that encapsulates the device's total power by accounting for qubit count, connectivity, gate fidelity, and coherence times. Circuit Layer Operations Per Second (CLOPS), which gauges how quickly a quantum processor can carry out layers of quantum operations, is another significant hardware-centric metric [23]. The device's throughput is measured by CLOPS, which is especially important for applications like variational quantum algorithms that need to execute numerous circuits. These metrics offer crucial context for interpreting the analysis's findings, even though QISAP does not directly use them in its machine learning models. For instance, a circuit that is expected to function well in practice is likely to have a high compiler_score on a device with a high QV.

2) Compiler-Centric Measures: Gate Counts and Circuit Depth: A quantum compiler's output quality is assessed using compiler-centric metrics. Since reduced resource requirements for circuit execution are frequently associated with better performance on NISQ devices, these metrics are usually centered on this goal. Gate counts and circuit depth are the most widely used compiler-centric metrics. Circuit depth is a proxy for the circuit's overall execution time and is defined as the length of the circuit's longest path, as covered in Section II. In general, a lower depth is preferable since it lessens the effect of decoherence. Since two-qubit gates are frequently the main cause of error on modern quantum devices, gate counts—in particular, the number of two-qubit gates—are also an important metric. A good compiler will try to reduce the number of two-qubit gates in the compiled circuit as well as their depth. The quantity of SWAP gates, which are frequently needed to map a circuit to a device with poor connectivity, and the total number of gates of each type in the device's native gate set are additional compiler-centric metrics. Many of these metrics are used by QISAP as features in its machine learning models, including depth, cx_count, and total_ops, as they accurately forecast the circuit's ultimate performance.

3) Application-Centric Measures: Success Probability and Fidelity: The best way to gauge the success of a quantum computation is through application-centric metrics. These metrics are specific and are defined in terms of the computation's final output to the running application. For instance, in a simulation of quantum chemistry, the pertinent metric might be the precision of the ground state energy calculation. Within a quantum machine learning classification task, it could be the accuracy of the classification. For a lot of quantum algorithms, like Shor's factoring algorithm or Grover's search, the pertinent metric is the likelihood of getting the right response following a single circuit run. Fidelity is another crucial application-centric metric that evaluates how "close" the circuit's actual output state is to the ideal, desired output condition. A gauge of the computation's overall quality, fidelity is a function of the compiler's circuit optimization skills as well as the noise in the hardware. Although application-centric metrics are not directly measured by QISAP, its objective is to forecast the compiler that, for a specific circuit and hardware combination, will optimize these metrics. These application-centric metrics are represented by the compiler_score in QISAP, and the platform's high prediction accuracy indicates a robust relationship between the compiler-specific metrics and the performance at the application level.

VI. Comparative Evaluation of Current Instruments

Quantum software is a rapidly developing field, with an increasing number of tools and frameworks being created to facilitate the design, analysis, and implementation of quantum circuits. It is crucial to compare QISAP with other tools that are currently available in this field in order to appropriately contextualize its contributions. This segment offers a comparative evaluation of QISAP with a number of other well-known quantum software frameworks, such as Qiskit Machine Learning, the MQT Predictor, and other specialized tools like Arline Benchmarks, QUARK, and QUANTIFY. The comparison highlights important elements like the feature extraction methodology, the machine learning models employed, the extent of the analysis, as well as the platform's overarching objectives. This analysis emphasizes the distinctive advantages of QISAP, especially its emphasis on compiler recommendation and utilization of a rich set of structural and information-theoretic metrics, while also pinpointing areas in which it can learn from and integrate with other tools.

A. Machine Learning with Qiskit

Qiskit Machine Learning is an extensive and popular framework for creating and executing algorithms for quantum machine learning [7]. It is included in the broader Qiskit ecosystem, which offers a comprehensive set of tools for quantum computing, ranging from hardware implementation

TABLE I: Comparative analysis of QISAP with other quantum software frameworks

Feature	**QISAP**	**MQT Predictor**	**Qiskit ML**
Primary Goal	Compiler recommendation and circuit analysis	Hardware selection prediction	Quantum machine learning algorithms
Core Technology	Classical ML (Random Forest)	Graph Neural Networks	Hybrid quantum-classical models
Feature Extraction	Manual (structural & info-theoretic metrics)	Direct DAG representation	Parameterized circuit parameters
ML Model	Random Forest Regressor & Classifier	Graph Neural Networks	Variational quantum circuits
Input Representation	Extracted metrics	Circuit DAG	Quantum circuit parameters
Output	Compiler recommendation, confidence score, visualizations	Device recommendation, performance prediction	Trained QML models, predictions
Key Strength	Interpretable features, high predictive accuracy, user-friendly interface	Full structural preservation, scalability	Deep integration with Qiskit ecosystem

to circuit design. With its extensive toolkit for building and training quantum neural networks and implementing other QML models, Qiskit Machine Learning is intended to be a versatile and expandable platform for QML research. Although both QISAP and Qiskit Machine Learning apply machine learning to quantum circuits, each has their own objectives and methods. Using classical machine learning to forecast compiler performance, QISAP focuses on the analysis and optimization of quantum circuits themselves. However, Qiskit Machine Learning focuses on using quantum circuits as part of a machine learning model to accomplish a particular task, like regression or classification.

1) Feature Extraction and Model Structures: Qiskit Machine Learning's feature extraction and model architectures are customized to meet QML's unique requirements. Usually, the features are the parameters of a parameterized quantum circuit, which are tuned to minimize a loss function throughout training. The models are frequently hybrid quantum-classical models, in which the input data is processed by a quantum circuit and the output is processed by a classical neural network. The classical optimizer uses the output of the classical neural network to update the parameters of the quantum circuit during the training process, which consists of a feedback loop between the classical and quantum components. Compared to QISAP, which employs a set of pre-computed structural and information-theoretic metrics as characteristics of a traditional machine learning model, QISAP aims to comprehend and forecast the behavior of a specific quantum circuit using various compilation techniques rather than train a quantum model.

2) Integration with Qiskit Ecosystem: The close integration of Qiskit Machine Learning with the larger Qiskit ecosystem is one of its main advantages. This enables users to easily transition between using Qiskit Terra to design a quantum circuit, Qiskit Machine Learning to train a QML model, and Qiskit Runtime to execute the model on an actual quantum device. This close integration offers QML developers and researchers a streamlined and effective workflow. In contrast, QISAP is a more independent tool, even though it parses OpenQASM files using Qiskit. Although QISAP might be incorporated into the Qiskit ecosystem, it is currently intended to function as a stand-alone platform with a unique workflow. A useful future path might be the incorporation of QISAP's compiler recommendation features into the Qiskit ecosystem, which would make it simple for Qiskit users to obtain data-driven suggestions for circuit optimization.

B. The MQT Predictor

Similar to QISAP, the MQT (Munich Quantum Toolkit) Predictor makes predictions about how well quantum circuits will function using machine learning [24]. But the MQT Predictor approaches the problem differently and with a different focus. The MQT Predictor focuses on predicting which quantum device would be best suited to run a particular circuit, whereas QISAP recommends the best compiler for a given circuit. In the NISQ era, where a wide variety of quantum devices are available, each with distinct properties and limitations, this is an important issue. The MQT Predictor seeks to offer data-driven suggestions for the best device to use for a particular circuit, assisting users in navigating this complicated environment.

1) Graph Neural Network Approach: The MQT Predictor's primary innovation is its direct learning from the quantum circuit's structure through the use of Graph Neural Networks (GNNs). The MQT Predictor represents the circuit as a directed acyclic graph (DAG) and feeds this graph straight into a GNN, as opposed to QISAP's method of extracting a set of manually created features from the circuit. After that, the GNN is trained to forecast the circuit's performance on various devices. The benefit of this method is that it can fully capture the circuit's structural information without requiring manual feature engineering. Because it can manage circuits of various sizes and configurations without requiring retraining, it also has the potential to be more scalable. In contrast to the more conventional machine learning method employed in QISAP, the application of GNNs is a potent and promising method for quantum circuit analysis.

2) Direct DAG Representation vs. Manual Feature Engineering: In quantum circuit analysis, there is a fundamental trade-off between the manual feature engineering method used

in QISAP and the direct DAG representation used in the MQT Predictor. Because it can capture all of the circuit's structural information, the direct DAG representation has the advantage of being more powerful and more general. But it also necessitates more complex machine learning models, like GNNs, and can be more computationally costly to run and train. However, because the features are selected using domain knowledge and are easily comprehensible by humans, the manual feature engineering approach is more straightforward and interpretable. Additionally, it makes it possible to employ more conventional and well-known machine learning models, like Random Forests. The particular objectives of the analysis and the resources at hand will determine which of these two methods is best. Although the direct DAG representation is a promising avenue for future research, the manual feature engineering approach was selected for QISAP due to its ease of use and interpretability.

C. Additional Analysis of Quantum Circuits Structures

The MQT Predictor and Qiskit Machine Learning are just two of the frameworks and tools that are pertinent to the study of quantum circuits. These tools frequently focus on more specialized tasks like optimization, profiling, or benchmarking. A synopsis of a few of these tools and their connection to QISAP are covered in this section.

1) QUARK: A Modular Benchmarking Framework: QUARK is a flexible and modular framework for creating application-level benchmarks in quantum computing [25]. Its main goal is to evaluate how well quantum algorithms and hardware perform across many different problems.

The framework has several building blocks, including: - Benchmark Manager (manages the benchmarking process), - Application module (represents the problem being tested), - Mapping module (handles how the problem is mapped onto a circuit), - Solver (runs the algorithm), - Device module (represents the target hardware).

Because QUARK is modular, it is easy to customize and extend. This makes it a strong tool for both researchers and developers.

Importantly, QUARK focuses on high-level evaluation of quantum applications, while QISAP focuses on low-level circuit analysis and optimization. Since they cover different layers of evaluation, the two tools complement each other and could even be combined to build a more complete benchmarking system.

2) QUANTIFY: A Cirq-based Analysis Tool: QUANTIFY is an open-source framework for analyzing quantum circuits [8]. It is built on top of Google's Cirq framework and provides tools for both analyzing and optimizing circuits. One of its features is semi-automatic circuit rewriting, which helps improve circuits automatically.

QUANTIFY also provides several circuit metrics, including: - T-count (the number of Clifford+T gates in a circuit), - Circuit depth (how many layers of operations the circuit has), - Number of CNOT gates (an important measure of complexity and cost).

These metrics are very similar to the ones used in QISAP. However, QUANTIFY is designed specifically for the Cirq ecosystem, while QISAP has a broader focus. Both tools operate at the low-level analysis of circuits, but each has different strengths and features.

3) Arline Benchmarks: A Cross-Platform Compiler Benchmarking Tool: Arline Benchmarks is an open-source package for automatically benchmarking quantum compilers [13], [14]. It is designed for the NISQ era and provides a dedicated way to profile and compare the performance of different quantum compilers.

Arline Benchmarks evaluates compilers using important metrics such as: - Post-optimization gate counts (the number of gates after the compiler optimizes the circuit), - Circuit depth (how many layers of operations remain after compilation), - Compiler run time (how long the compiler takes to finish its job).

One of its unique ideas is the composite compilation pipeline. This means combining optimization routines from different compilers into a single workflow, so the final compilation benefits from the strengths of multiple compilers.

Arline Benchmarks is closely related to QISAP since both are concerned with quantum compilers. However, there is a key difference: - Arline Benchmarks focuses on benchmarking compilers themselves, - QISAP focuses on recommending the best compiler for a given circuit.

Because of this, the two tools are complementary and could even be integrated into one system for both benchmarking and recommending compilers.

VII. Limitations and Future Work

Although the Quantum Integrated System Analytics Platform (QISAP) represents a substantial advancement in the use of machine learning in quantum circuit analysis and compiler recommendations, it has limitations. The present implementation serves as a proof-of-concept to show how effective this strategy can be. However, it can be expanded and enhanced in a number of areas. This section explains the current QISAP platform's known limitations and provides a roadmap for upcoming improvements and lines of inquiry. Among these potential paths are enhancing the machine learning models' resilience, adding more advanced quantum-aware metrics, and broadening the platform's reach to encompass a greater variety of technologies and applications related to quantum computing.

A. Current Limitations of QISAP

There are a number of issues with the current QISAP version that are recognized in the documentation for the project. These restrictions mostly pertain to the dataset that was utilized for the machine learning model training, the extent of the circuit representation, and the analysis's static character. One of the top priorities for the future development of the platform is to address these limitations.

1) Impact of Outlier Circuits on Model Performance: The sensitivity of the current QISAP implementation to outlier circuits is one of its primary drawbacks. Although the dataset of 168 quantum circuits used to train the machine learning models is diverse, it does contain some extreme examples that may distort the regression models. Outlier circuits like *factor247_n15.qasm* and *bwt_n177.qasm* have structural characteristics that differ significantly from those of most circuits in the dataset [15], [26]. Because of this, regression models may find it challenging to forecast how well these circuits will perform, and their inclusion in training data may have an adverse effect on the models' overall performance on more common circuits. This issue is prevalent in machine learning and emphasizes the need for stronger modeling strategies that can deal with outliers more tactfully.

2) Limited QASM 3.0 Support: The current QISAP platform's limited support for the OpenQASM 3.0 standard is another drawback. Although OpenQASM 2.0 is a widely used standard, the platform is currently made to work with files that lack some of the newer version's features. OpenQASM 3.0 introduces several new features, including classical control flow, pulse-level definitions, and a wider variety of data types, which are necessary to fully utilize the capabilities of contemporary quantum hardware and to describe increasingly complex quantum algorithms [27]. The circuit types that QISAP can analyze are restricted by its lack of support for QASM 3.0, which also makes it incompatible with some of the newest frameworks and tools for quantum programming.

3) Static Dataset and Lack of Real-Time Circuit Upload: The QISAP platform currently in use is made to operate with a static dataset of pre-compiled circuits. The machine learning models are trained using the metrics that are taken out of these circuits and saved in a CSV file. Although this method works well for proof-of-concept, it lacks flexibility and scalability. If users could upload their own circuits for real-time analysis, that would be far more helpful. Instead of being restricted to the circuits in the given dataset, this would enable researchers and developers to use QISAP to analyze and optimize their own quantum algorithms. QISAP would be a far more useful and practical tool for the quantum computing community if it could upload circuits in real-time.

B. Future Enhancements and Research Directions

In order to overcome QISAP's present shortcomings and increase its functionality, there are numerous possible directions for further study and advancement. These improvements range from strengthening the machine learning models' resilience to incorporating more sophisticated quantum information-theoretic measurements and broadening the platform's application to encompass a greater variety of applications for quantum computing.

1) Advanced Outlier Handling and Separate Modeling: One possible way to deal with the issue of outlier circuits is to add more sophisticated methods for handling outliers. Using reliable regression models that are less susceptible to outliers may be necessary for this, or it might entail locating and eliminating outliers from the training data prior to model fitting. An alternative strategy would be to create distinct models for various circuit classes. For instance, one could use a clustering algorithm to divide the circuits into various groups according to their structural characteristics, after which each cluster's unique regression model is trained. This would enable the models to focus on forecasting the performance of a specific kind of circuit, which might result in predictions that are generally more accurate.

2) Integration of Quantum-Aware Metrics: The existing QISAP platform makes use of a traditional information-theoretic metric called *instruction_entropy* to describe quantum circuit complexity. This metric is helpful, but it doesn't fully capture the information's quantum nature. A promising avenue for future research is adding more sophisticated, quantum-aware metrics to the platform, like pseudo-entropy and linear entropy [5], [6]. These measurements, which are grounded in the ideas of quantum information theory, can offer a more complex and precise description of quantum circuit characteristics. Combining these metrics would necessitate more advanced computational techniques, but it might result in a notable enhancement in the machine learning models' capacity for prediction.

3) Compiler-Specific Optimization Suggestions: At the moment, QISAP recommends a compiler to use for a specific circuit, but it doesn't offer any detailed recommendations on how to make the circuit better for that compiler. A useful addition in the future would be to include a function that offers recommendations for compiler-specific optimization. This might entail examining the composition of the circuit and determining particular adjustments or enhancements that could be implemented to enhance its functionality on the suggested compiler. As an illustration, the system might propose an alternative gate decomposition, a different qubit mapping, or the inclusion of sequences of dynamical decoupling. QISAP would become a far more potent tool for circuit optimization since it would give users specific, useful guidance for enhancing their circuits.

4) Expansion to Fault-Tolerant Quantum Computing (FTQC) Metrics: Right now, the QISAP platform is mainly built for the NISQ era of quantum computing. In this era, the main challenge is noise and decoherence, so the focus is on keeping their effects as small as possible.

But as quantum computing advances into the era of fault-tolerant quantum computing (FTQC), the way we evaluate circuits will have to change. In FTQC, the focus will no longer just be on reducing noise [2], [18]. Instead, the big challenge will be handling the overhead that comes from quantum error correction.

This shift brings in a different set of metrics, such as: - **Logical error rate** – the probability that an error remains even after error correction. - **Code distance** – a measure of how well the error-correcting code protects information. - **T-count** – the number of non-Clifford gates (which are costly to implement in error-corrected circuits).

A long-term vision for QISAP would be to expand and include these FTQC metrics. This would make the platform useful not only for today's noisy quantum computers but also for analyzing and optimizing fault-tolerant quantum algorithms in the future. While this would require significant development, it would ensure that QISAP continues to stay relevant and valuable as quantum computing moves forward.

VIII. Conclusion

The Quantum Integrated System Analytics Platform (QISAP) represents a significant contribution to the field of quantum computing, offering a thorough and practical framework for quantum circuit analysis and optimization. Using classical machine learning methods, QISAP can forecast the performance of various compilers on a specific circuit with a high level of precision, allowing users to choose a compiler based on data. The platform is a useful resource for researchers and practitioners in the field of quantum computing because of its extensive feature set, which includes an interactive dashboard, automated report generation, and a compiler recommendation system.

A. Summary of Contributions

This paper makes three major contributions. First, we have presented a wide range of metrics, including the new *instruction_entropy* metric, for describing the information-theoretic and structural characteristics of quantum circuits. We have examined this metric's implications for comprehending circuit complexity and offered a thorough mathematical analysis. Second, we have demonstrated a strong machine learning pipeline that makes use of these metrics to provide high predictive accuracy for compiler performance. The R2 score of our regression models is roughly 0.95 for predicting a proxy for compiler performance, indicating the strong relationship between circuit structure and compilation results. Third, we have created a useful and intuitive compiler recommendation system that offers not just a suggested compiler, but also a complete probability distribution across all available compilers and a confidence score. Based on the model's predictions, this system enables users to make well-informed decisions.

B. Impact on the Quantum Computing Community

The quantum computing community could be greatly impacted by the QISAP platform. By offering a data-driven method for choosing a compiler, the time and effort needed to optimize quantum circuits can be decreased with the aid of QISAP, which is a significant obstacle to the advancement of quantum applications. From students and educators to seasoned researchers and developers, a broad spectrum of users can access the platform thanks to its interactive dashboard and automated reporting system. QISAP can assist in simplifying and facilitating the analysis of quantum circuits, helping to quicken the rate of quantum computing research and development.

C. Final Remarks

To sum up, the Quantum Integrated System Analytics Platform (QISAP) is an effective and adaptable instrument for quantum circuit analysis and optimization. It is a useful addition to the quantum software ecosystem because of its distinctive blend of a robust machine learning pipeline, a rich set of metrics, and an intuitive user interface. Although there are still a few issues to be resolved and a lot of fascinating avenues for further research, the current QISAP implementation shows how machine learning can be used to address the intricate problems of quantum circuit compilation. We think QISAP will be a useful tool for the field of quantum computing and will contribute to the creation of more potent and effective quantum applications.

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