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Generic Quality Control Tool for Environmental Marine Datasets

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***Abstract-** In order to ensure the reliability and accuracy of Marine observation data, there is a need to make sure that the data are reliable and of good quality. This is important because in situ datasets obtained via observation platforms are usually subject to measurement errors, faulty instruments, failed communications, and environmental disturbances, which leads to data corruption and misinterpretation. In this paper, a Generic Quality Control Tool for Marine Observation Datasets that automatically determines anomalies in time series is proposed. The framework incorporates several quality control methods, including range testing, spike detection, and stuck value determination. It is implemented in Python language, with the use of Pandas library. The system assigns each record a quality flag depending on the set validation criteria and helps in distinguishing invalid observations from valid ones. The system can be easily customized for different types of environmental variables, including sea surface temperature, salinity, and wave height. The experimental results show the effectiveness of the proposed tool. The proposed system provides a scalable and efficient tool for quality assessment on an automated basis, which will help to increase the reliability of data and environmental monitoring systems.*

I. INTRODUCTION

The Ocean covers about 71 percent of the surface area on Earth and plays an important part in managing the Earth's climate, Marine ecosystem, and environmental sustainability. The oceans serve as huge reservoirs of heat and carbon affecting weather systems, ocean circulation, and global climate systems. Ocean dynamics thus play a vital role in understanding climate change, Marine resources management, disaster forecasting and monitoring [15]. To reach this goal, a huge amount of data from oceans is continuously being gathered through different types of observation platforms and systems all around the world.

Modern ocean observing systems have in-situ and remote sensing components. In-situ systems include moored buoys, drifting buoys, Argo floats, and tide gauges, providing information on the state of the ocean directly, whereas remote sensing platforms like satellites cover huge areas of the Marine environment [2], [15]. Observation systems collect huge volumes of data in the form of time series related to different parameters of the Marine environment such as sea surface temperature, salinity, wave height, sea level, ocean currents, and atmosphere [17], [31]. Though there have been considerable advancements in the field of ocean observing technology, preserving the quality and accuracy of the observed data has remained to be a challenging task. The Marine data sets can be compromised due to many factors of errors caused by degradation, calibration errors, biofouling, communication problems, environmental disturbances, and processing errors [7], [10], [23]. Harsh conditions of the Marine environment can compromise the performance of the sensors, causing incorrect measurements and erroneous observations. Moreover, transmission errors, and errors in storage may cause problems like missing values, duplicated observations, and corrupted observations in the data set [13], [14].

As the Marine observations are collected as time series data, they are highly prone to errors which can negatively affect the results and decision making processes later on. Some common anomalies found in ocean data include outlier data, spikes, jumps, missing values, and stuck values as a result of malfunctioning of the sensors or communication problems [1], [8], [21]. Such anomalies can cause incorrect scientific findings, erroneous forecasting models, and poor decisions, therefore, preserving the quality of the data before analysis has become imperative in today's world [24], [39]. QC methodologies are commonly applied in order to evaluate the validity and consistency of the observational data prior to its further use for scientific and operational applications. International programs for ocean observation like Argo program, World Ocean Database (WOD), and

IQuOD (International Quality-Controlled Ocean Database) provide standard QC procedures that aim at improving reliability and compatibility of data coming from various observation networks [17], [31], [39]. These procedures usually incorporate automated and manual inspection strategies in order to detect dubious observations and assign appropriate quality flags to each measurement.

Traditional quality control strategies include range test, climatological test, spike test, gradient test, and temporal consistency test [2], [23], [30]. The range test ensures physical acceptability of the observations, and spike test detects abrupt abnormal changes in the data. Climatological test is aimed at comparing the observed value with historical environmental conditions, whereas temporal consistency test guarantees the realism of observations' time trend. All of these strategies demonstrated their efficiency in detecting data problems and are widely used nowadays [18], [40]. A number of recent studies have investigated the use of machine learning algorithms, statistical models and anomaly detection algorithms in automation of quality assessment process [8], [16], [21], [42]. Modern approaches like outlier detection, pattern recognition and change-point analysis have proven their capability to detect complex anomalies in environmental time-series data [4], [20], [27], [37].

With the purpose to solve these problems, this paper introduces the Generic Quality Control Tool for Marine Datasets, which can be used for automatic detection and flagging of anomalous observations in time series data on oceans. Proposed method incorporates multiple quality control algorithms, namely Range Tests, Spike Tests and Stuck Value Tests into one scalable system.

Proposed tool is aimed at providing high flexibility, which enables its application to different Marine parameters (e.g. temperature, salinity, wave height). The combination of multiple quality control algorithms within one system makes it possible to increase integrity of data, reliability of its scientific analysis and usability of ocean observation datasets. The results prove efficiency of the proposed approach in detection of different types of anomalies.

II. RELATED WORK

Quality of Environmental Monitoring observations is a key research topic due to increasing reliance on the ocean data in the climate studies, Marine forecasting and environmental observations. Several research papers suggested quality control approaches for identification and removal of erroneous ocean data. Bailey et al. [2] introduced standard quality control for Marine observations, stressing the need of automated validation approaches. Similarly, Ingleby and Huddleston [23] suggested quality control approaches for ocean temperatures and salinity profiles obtained using observational platforms.

There are international Marine observing systems (Argo and World Ocean Database), which apply automated and manual quality control approaches to improve data reliability [17], [39]. Morello et al. [30] developed quality control approaches for Australian Integrated Marine Observing System and Xu et al. [40] developed automated quality control approach for Marine profile observations.

There is also extensive use of anomaly detection approaches in the analysis of environmental and Marine data. Chandola et al. [8] gave a survey of existing anomaly detection approaches, while Hill and Minsker [21] illustrated anomaly detection approaches for environmental sensor data. In recent times, various machine learning techniques have been investigated to develop techniques for quality control and anomaly detection in Marine datasets [16], [42]. While these techniques enhance detection accuracy, they often require a vast amount of data for training and computation power.

Previous works have mainly concentrated either on particular datasets or particular quality control tests. Hence, there is a requirement for developing a generic scalable framework where a variety of quality control tests can be integrated. The proposed work attempts to meet this requirement by incorporating Range, Spike, and Stuck Value Tests under one umbrella of quality control technique.

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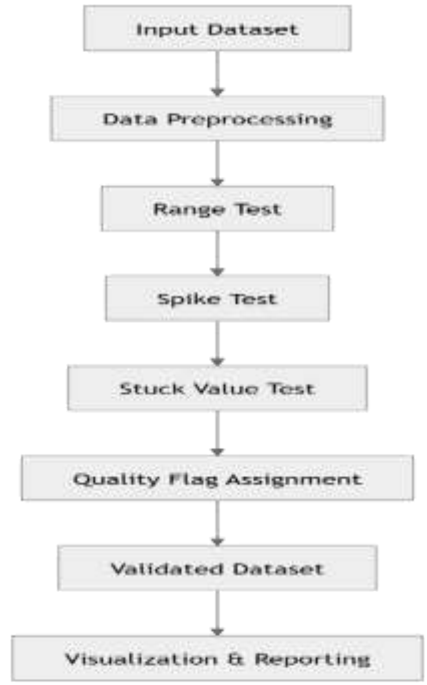
III. PROPOSED METHODOLOGY

The main aim of the work under consideration is to design a generic and automated quality control system able to detect abnormal readings within the time-series of Marine observations. Environmental observing systems constantly accumulate vast amounts of environmental information through sensors placed in dynamically changing Marine environment. These readings may be influenced by factors such as sensors wear and tear, calibration problems, environment impact, data transmission problems, and processing errors. All these aspects create discrepancies which negatively affect the reliability of any analysis and decision-making process. Thus, the need for effective quality control system becomes apparent. A proposed Generic Quality Control Tool represents a system with a systematic and modular approach to assessing data quality. The tool takes Environmental Monitoring time-series as its input and performs several quality control operations in order to detect suspicious readings. At first, the raw data goes through several preprocessing operations, such as conversion of timestamps, missing data handling, duplicates removal, and chronological ordering. In addition to preprocessing, there are three complementary quality control procedures in the proposed framework that include the Range Test, Spike Test, and Stuck Value Test. The Range Test is a check of the observations against physical limitations and detection of impossible observations. Spike Test detects the sudden abnormal changes between two consecutive values in the time series data set. These spikes might be caused by sensor noises, communication issues, or temporary malfunction of equipment. The comparison between two neighboring observations is done and any measurement above a certain threshold value is marked as suspicious.

Stuck Value Test determines instances when a certain value keeps repeating itself in a data set. These instances may be caused by freezing of sensors, incorrect calibration, or communication issues. Any repeated value above a certain threshold is flagged as suspicious. The use of these tests provides an opportunity to detect various errors resulting from sensor failure, communication problem, and environment impact.

For more convenient usage of the system, a flagging system was developed for classification of the observations as valid, suspect or invalid on the basis of the quality control tests' outcomes.



Moreover, visual inspection methods were included into the process for better anomaly detection and interpretation. The proposed framework is flexible and can be scaled to be used for any number of observations and Marine parameters such as temperature, salinity, wave height and sea level, etc. Workflow of the Generic Quality Control Tool. The process starts from data collection and pre-processing, and further proceeds to the implementation of quality control tests. According to the results of the tests, quality flags are created and the validated data set is produced. The final product includes quality-controlled observations and visualizations that help researchers evaluate the reliability of Marine data.

IV. ALGORITHM FOR GENERIC QC FOR MARINE DATA

Input: - Marine time series data ($D\ \{x1, x2, \ldots, xn\}$)
Output: - Quality controlled dataset with quality flags.
Step 1: Data pre-processing
1. Data set is loaded
2. The timestamps are converted to datetime format.

3. The observations are sorted chronologically.
4. Duplicate entries are removed.
5. Missing data entries are dealt with

Let: -

$$[D = \{x1, x2, x3, \ldots\ldots, xn\}]$$

where (xi) is an observation at time (ti)

Step 2: Range Test

The aim of the Range test is to check if all observations fall within specified physical limits.

Let:-

L=Lower Physical Limit

U = Upper Physical Limit

For each observation x_i:

$$L \leq x_i \leq U$$

If the condition is satisfied:

Flag(x_i) = Good

Otherwise:

Flag(x_i) = Bad

$$[L = \backslash text\{Lower\ Limit\}]$$
$$[U = \backslash text\{Upper\ Limit\}]$$

For each observation (x_i),

$$[L \backslash leq\ x\_i \backslash leq\ U]$$

If the above holds true

$$[Flag(x\_i) = Good]$$

Else

$$[Flag(x\_i) = Bad]$$

For example, for Sea surface temperature

$$[0\text{^}\backslash circ\ C \backslash leq\ SST \backslash leq\ 40\text{^}\backslash circ\ C]$$

Any data point outside this limit is flagged as bad.

Step 3: Spike Test

The Spike Test detects abrupt abnormal differences between adjacent measurements.

For each measurement:

$$Spike_i = |x_i - ((x_{i-1} + x_{i+1})/2)|$$

If

$Spike_i > T_s$

where T_s is the spike threshold,

the observation is flagged as anomalous.

$$[Spike\_i = \backslash left|x\_i - \backslash frac\{x\_\{i-1\} + x\_\{i + 1\}\}\{2\}\backslash right|]$$
$$If:$$
$$[Spike\_i > T\_s]$$

with (T_s) being the threshold for spikes, then the measurement is marked as an anomaly.

Otherwise:

$$[Flag(x\_i) = Good]$$

This test assists in detecting sensor noise and transmission problems.

Step 4: Stuck Value Test

The Stuck Value Test detects situations when sensors get stuck to a single value for a long period of time.

For a sequence of measurements:

$x_i = x_{i+1} = x_{i+2} = \ldots = x_{i+k}$

If

$k > K$

where K is the maximum allowable repetition count,

Flag(x_i) = Suspect

$$[x\_i = x\_\{i+1\} = x\_\{i+2\} = \ldots = x\_\{i+k\}]$$

If the count of repetitions is higher than (K):

$$[k > K]$$

Then

$$[Flag(xi) = Suspect]$$

Step 5: Quality Flag Assignment

Considering the results of all tests,

Flag	Explanation
1	Good Data
2	Suspect Data
3	Bad Data

For every data point,

Q_i = f(Range Test, Spike Test, Stuck Value Test)

where Q_i represents the final quality flag assigned to observation x_i.

$$[Q\_i = f(Range, Spike, Stuck)]$$

Here, (Q_i) is the assigned quality flag.

Step 6: Produce the Output

Store the quality flag in the data.

Remove/Filter out invalid observations.

Produce graphical representation of the anomalies.

Export the validated data set. Algorithm Complexity

Considering the case where there are (n) observations in the data set,

$Range\ Test:\ (O(n))$

$Spike\ Test:\ (O(n))$

$Stuck\ Value\ Test:\ (O(n))$

Complexity of the Algorithm :$[O(n)]$

So, it can be seen that the developed quality control algorithm works effectively on large scale Marine data sets

V. PERFORMANCE METRICS

The effectiveness of the developed Generic Quality Control Tool is measured using both anomaly detection performance and computational performance indicators. The described measures present numerical proof of the capabilities of the system in terms of accurate detection of anomalous observations along with effective processing of large Marine datasets. As the ocean monitoring systems produce large quantities of time-series data on a continuous basis, both aspects have to be considered to improve the quality of Marine datasets.

Detection Accuracy
The Detection Accuracy indicator shows the level of overall accuracy of the process of anomaly detection. This is the measure of proportion of observations that have been successfully recognized as normal or anomalous.

$$Accuracy = (TP + TN) / (TP + TN + FP + FN)$$

where:
TP (True Positive): detected anomalies;
TN (True Negative): detected normal observations;
FP (False Positive): normal observations which have been detected as anomalies;
FN (False Negative): missed anomalies.
High value of this indicator proves that the developed system recognizes valid and invalid observations effectively.

Precision
The Precision indicator is a measure of reliability of the process of anomaly detection and is defined as the measure of proportion of true anomalies among all detected anomalies.

$$Precision = TP / (TP + FP)$$

The greater the value of Precision, the less number of false alarms and the better the identification of suspicious data by the system is. The precision is especially important for Marine quality control since the false alarms can lead to the discarding of good data about environment.

Recall
Recall, or True Positive Rate (or Sensitivity) evaluates the ability of the framework to detect all anomalies existing in the dataset.

$$Recall = TP / (TP + FN)$$

The great value of Recall means that most anomalous data are detected. Recall is essential in oceanography because the non-detected anomalies will affect further analysis, forecasting, and decision-making.

F1-Score
F1-Score is the combined measure of Precision and Recall. It gives us the balanced evaluation of the performance of the anomaly detection in the case of the uneven distribution of normal and anomalous data.

$$F1 - Score = 2 \times (Precision \times Recall) / (Precision + Recall)$$

The higher the F1-Score, the higher the precision and recall achieved by the system, hence a reliable measure of anomaly detection.

False Positive Rate (FPR)
False Positive Rate indicates the percentage of non-anomalies falsely marked as anomalies.

$$FPR = FP / (FP + TN)$$

The lower the value, the more reliable the system performance and less risk of losing valuable data. Avoiding false positives is key to ensuring integrity of Marine data sets.

Execution Time The Execution Time indicates the time taken to perform the quality control procedure on the data set. The formula for calculating Execution Time is:

$$Execution\ Time = T_{end} - T_{start}$$
$$Where:$$
$$(T\_\{start\})\ is\ the\ starting\ time\ of\ processing.$$
$$(T\_\{end\})\ is\ the\ finishing\ time.$$

The lower the execution time, the better computational efficiency and hence ability to process large data sets in near-real-time environment.

Memory Utilization
Memory Utilization refers to the system memory utilized in performing quality control tasks. Memory efficiency becomes critical in case of long term ocean observation where there will be millions of data records.

$$[Memory\backslash\ Utilization = Memory\_\{used\}]$$

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Lower memory usage enhances scalability and ensures that the framework functions properly under conditions of limited computational power.

Scalability Analysis

Scalability can be defined as the ability of the framework to sustain its performance despite the growing size of the data set. As all tests (Range Test, Spike Test, Stuck Value Test) run their observations one by one, the computational complexity of each test is estimated as follows:

[O(n)]

where (n) denotes the number of observations within the dataset.

Therefore, the overall computational complexity of the framework is linear, which makes it appropriate for large-scale Marine data processing tasks.

Performance Evaluation Summary

The proposed quality control framework is measured according to such criteria as Accuracy, Precision, Recall, F1-Score, False Positive Rate, Execution Time, Memory Utilization, and Scalability. These measures are used to estimate the performance of the proposed method in terms of anomaly detection and computational efficiency.

VI. RESULTS

The suggested Generic Quality Control Tool was implemented using the Python programming language and tested on the Marine time series datasets including environmental variables such as sea surface temperature, salinity, and waves. The design of the framework allowed for automatic detection of anomalies and assignment of quality flags for suspicious observations. It was demonstrated in the experiment that the proposed solution is able to recognize different types of data quality problems efficiently and still be computationally effective for big datasets.

Firstly, the effectiveness of the Range Test was evaluated in the experiment. It was proven that the test could recognize observations violating the given physical constraints and those observations that do not represent realistic Marine values.

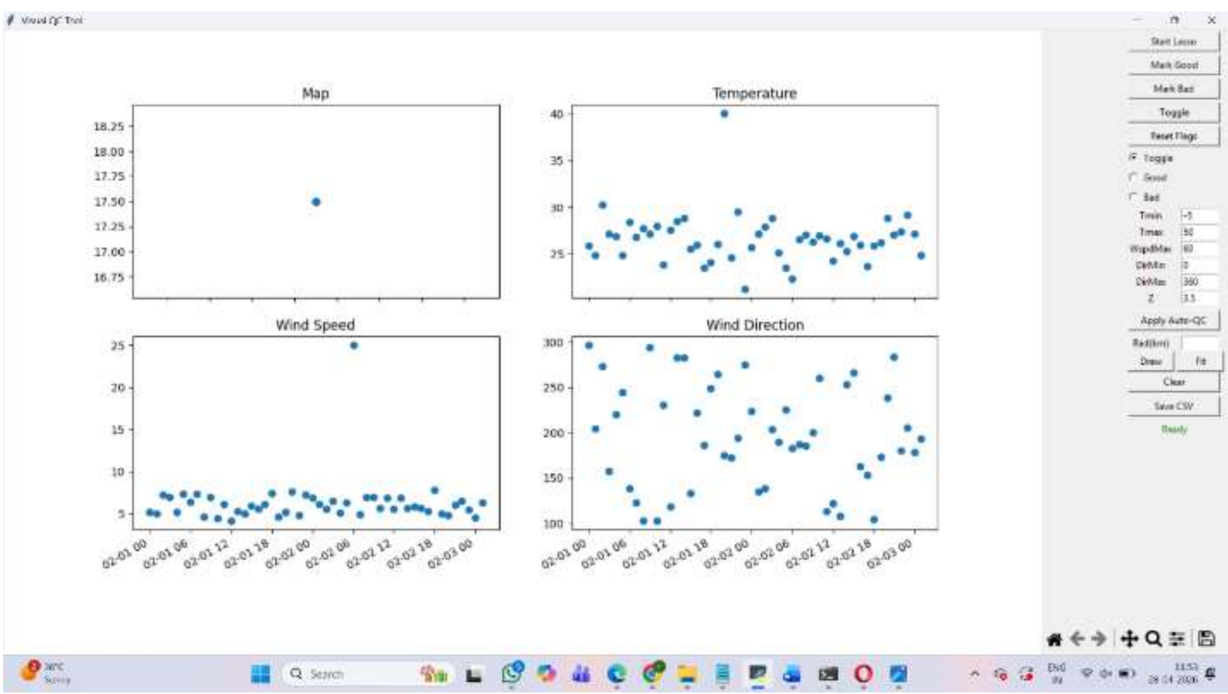

Fig. 2. Raw Dataset Before Quality Control

As it was mentioned earlier, the range based validation is widely used in operational oceanography since it allows for easy detection of gross measurement errors [2], [23], [39]. Thus, it was proved that the Range Test

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is an important first level screening approach for the elimination of physically impossible observations from the dataset.

For detection of spikes and sudden changes of values in the time series, the Spike Test was applied.
The ability to detect these short-term anomalies becomes crucial due to the distortion of statistics and forecasting that this type of measurement can create. This phenomenon has been observed earlier in the studies with environmental sensor networks and ocean monitoring systems [8], [21], [42]. The identified spikes were correctly classified as anomalies and separated from other measurements, increasing the data consistency. In order to find out the periods when the sensor reading was constant for an untypically long period of time, the Stuck Value test was applied. In most cases, such behavior of a sensor is caused by sensor freezing, incorrect calibration, and/or communication issues. Experimental results confirmed the ability of the proposed framework to identify repeated measurements and assign proper quality flags. This feature is particularly useful for long-term monitoring of the ocean when the degradation of the sensor can be unnoticed for a long time [18], [40].

The combination of several quality control procedures greatly improved the performance of the anomaly detection algorithm.

While each test was successful in identifying different types of anomalies, using all three Range Test, Spike Test, and Stuck Value Test allowed for a thorough examination of the data. The quality flags, which had been calculated during this procedure, allowed for classification of the observations in valid, suspect, and invalid observations, making it easier for users to remove unreliable observations before further analysis. This tier-based method of validating the data coincides with the guidelines set out by international ocean data quality control standards and operational ocean observing programs [17], [24], [31].

Furthermore, visualization of the datasets after the processing allowed confirming the effectiveness of the proposed framework. The graphical representation of the time-series data visually represented the abnormalities that had been found and the improvements in data consistency due to the data quality control procedures. As shown by the visual inspection results, abnormal observations that had been found by the proposed framework were very close to suspicious observations in the raw dataset.

As for the computational performance, the implementation using the Pandas library worked well for processing large datasets while still having low memory usage.

Because each quality control check algorithm involves sequential processing of data points, the general computational complexity of the approach stays O(n), which makes the framework applicable for real-time analysis and large-scale computations.

Scalability of the approach lets it be used for different Marine parameters without any significant changes to the framework itself.

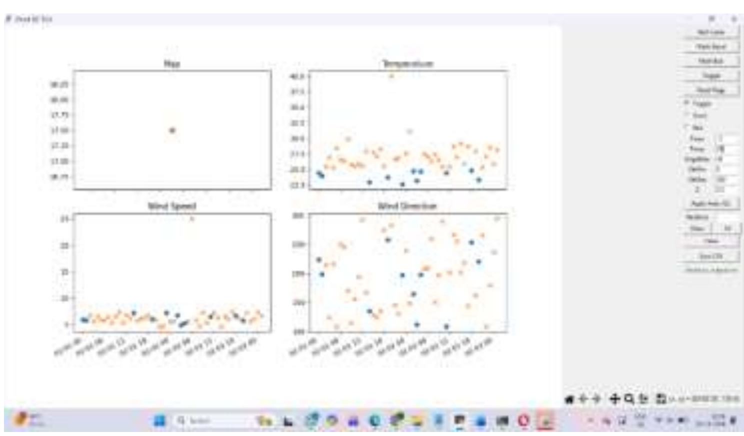

Fig. 3. Quality-Controlled Dataset After Applying QC Tests

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As it can be seen from the above experimental results, the developed Generic Quality Control Tool is able to provide considerable improvement of the reliability, consistency, and usability of Marine datasets. In comparison with single-tests approaches that were traditionally used before, the introduced approach offers a more complete tool for anomaly detection and data validation purposes.

Automated quality control checks, quality flags generation, and visualization features increase the data integrity and allow performing precise scientific analysis, environmental monitoring, and ocean forecasts [6], [18], [40].

Thus, experimental results confirm the scalability, efficiency, and effectiveness of the proposed approach for automatic quality control of Marine time-series datasets.

The developed quality control framework exhibited satisfactory anomaly detection abilities in all types of data quality problems. Specifically, the Range Test was successful in identifying observations that were beyond certain predefined physical thresholds, whereas the Spike Test was able to detect unusual abrupt changes that occurred due to sensor noise and transmission errors. In addition, the Stuck Value Test was successful in detecting repeated observations caused by freezing of sensors.

The generated quality flags ensured successful classification of observations into valid, suspicious, and invalid classes. It is evident from visual analysis of the cleaned datasets that the proposed framework improved data consistency and decreased the number of anomalous observations. Moreover, the development of the framework using Python and Pandas ensured efficient processing of large datasets. In the future, a comprehensive quantitative analysis will be performed using Accuracy, Precision, Recall, and F1-Score metrics.

VII. FUTURE WORK

Though the suggested framework demonstrates successful automated quality control employing rule-based validation techniques, there are still areas where improvements and developments can take place. In the future, the work is going to be devoted to applying the techniques of machine learning and artificial intelligence to increase the efficiency of anomaly detection.

Machine learning techniques are capable of learning complicated patterns from past observations and detecting anomalies that cannot be found using simple threshold-based methods [16], [42].

Change-point detection is another approach that is expected to be applied in the future for identifying structural changes and trends of Marine time series data. Change-point analysis can provide extra information on the behavior of sensors and environment thus increasing the effectiveness of the process of anomaly detection [27], [37].

The future versions of the framework are going to apply climatological and statistical consistency tests comparing observations with historical environment records. This will give a possibility of more thorough validation taking into account seasonal variations and regional oceanography [13], [32], [33]. Incorporating adaptive thresholds according to the environmental conditions may add additional robustness to the quality control process. Further, the developed algorithm can be utilized to analyze data streams collected from operational ocean monitoring systems in real-time mode. In this way, it is possible to detect abnormalities right after data collection, thus ensuring quick response to potential sensor malfunctions [18], [40].

Moreover, combining the proposed technique with cloud computing architectures and Internet of Things (IoT) infrastructure may lead to improved scalability and easy deployment of the framework in observation networks.

In the future, there will also be a need to develop an interactive dashboard that allows one to visually evaluate data quality and manually validate observations if necessary.

Finally, the described quality control framework can be easily generalized and applied for quality analysis of other environmental datasets.

This will enhance the use of the framework and aid in the development of a unified solution for quality control of the environment observation and Earth observation applications.

To sum up, future developments with machine learning, change point detection, real-time analysis, cloud implementation, and visualization have a great potential of enhancing the effectiveness of the suggested quality control framework in the next-generation ocean observation system.

VIII. CONCLUSION

The increase in Marine observations collected from in-situ instruments, monitoring stations, and environmental observation systems has led to a higher need for efficient data quality assurance solutions. Due to frequent failures in sensing mechanisms, communication, environmental disturbances, calibration issues, and data communication, the process of quality control has become an essential part in guaranteeing the validity and correctness of any analysis and practical use of data [2], [17], [24].

The purpose of this research was to develop a Generic Quality Control Tool for Environmental Monitoring, where a variety of quality control processes were united within one scalable solution. The system was designed to automatically recognize abnormal observations and set quality flags for particular observations to indicate their reliability. The tool uses Range Tests, Spike Tests, and Stuck Value Tests to estimate observations considering their physical, temporal, and operational aspects. The Range Test proved itself to be an effective procedure to identify observations beyond the defined physical boundaries and find unreal environmental data. The Spike Test was very useful in detecting sudden changes that occurred due to noise from sensors, data transmission errors, and temporary failures of the sensors. This helped the framework enhance the quality of the data set by minimizing the influence of outliers in the usefulness of Spike Test was very great in identifying changes that resulted due to noise in the sensors, transmission error in data and failure of sensors for a period of time. This was very useful in improving the quality of data set as it decreased the impact of abnormal data on the results. Likewise, the Stuck Value Test revealed long intervals of constant observations, which is characteristic for sensor freezing or communication issues. Combining these complimentary techniques helped perform a comprehensive data quality assessment and enhanced the performance of anomaly detection compared to using each test separately [18], [23], [39].

The usage of the proposed methodology implemented in Python language together with the Pandas library showed that it is possible to process large Marine datasets effectively while keeping the computational complexity at a low level. Quality flags were created to classify observations into the valid, suspect, and invalid types, and thus helped to perform an efficient data filtering and validation. The visualization of the processed datasets verified that the proposed system can identify anomalous observations successfully.

Thus, experimental verification proved that the proposed system increases the reliability, consistency, and usability of the Marine datasets. It was shown that combining several quality control techniques in one framework provides an efficient solution for automatic anomaly detection and data validation. Therefore, the proposed tool can be used for various scientific and operational Marine applications that require high-quality observational data [6], [31], [40].

In general, the development of the Generic Quality Control Tool offers an effective, flexible, and scalable way to automate the quality assessment process of Marine data. Thanks to improved quality of collected data, the framework facilitates better environmental analysis and meets modern needs of ocean observation systems.

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