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# SYSTEMS AND METHODS FOR DETERMINING TEST RESULT ACCURACIES IN DIAGNOSTIC LABORATORY SYSTEMS


## Abstract

A method of determining the accuracy of a test performed by a diagnostic laboratory system includes obtaining one or more first measurements during a first operation of the test performed by the diagnostic laboratory system. One or more second measurements are obtained during a second operation of the test performed by the diagnostic laboratory system. The first measurements and the second measurements are collectively analyzed using a trained model that calculates an uncertainty score for the test based on learned correlations between the first operation and the second operation. The uncertainty score may be used to determine whether the test results can be relied upon or whether the test should be rerun. Other methods and systems are disclosed.



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## Background/Summary

CROSS REFERENCE TO RELATED APPLICATION [0001] This application claims the benefit of U.S. Provisional Patent Application No. 63/374,885, entitled “SYSTEMS AND METHODS FOR DETERMINING TEST RESULT ACCURACIES IN DIAGNOSTIC LABORATORY SYSTEMS” filed Sep. 7, 2022, the disclosure of which is hereby incorporated by reference in its entirety for all purposes.

FIELD

[0002] Embodiments of the present disclosure relate to determining test result accuracies in diagnostic laboratory systems.

BACKGROUND

[0003] Clinical diagnostic laboratory systems process patient samples such as blood serum, blood plasma, urine, interstitial liquid. cerebrospinal liquids, and the like to obtain test results. The test results are subsequently used by clinicians to screen, diagnose, and/or monitor different patient conditions and diseases. Each test includes a plurality of different operations, such as aspirating the samples and adding reagents to the samples. Additionally, different types of tests perform operations in different sequences. If any operation fails during a test and the failure is undetected, the undetected failure can have a significant impact on the test result and any clinical decision made based on the test result. Therefore. a need exists for determining the accuracy of tests performed by diagnostic laboratory systems.

SUMMARY

[0004] In some embodiments, a method of determining accuracy of tests performed by a diagnostic laboratory system includes (a) obtaining one or more first measurements during a first operation performed by the diagnostic laboratory system, wherein the first operation is one of a plurality of operations used to perform a first test on a sample; (b) obtaining one or more second measurements during a second operation performed by the diagnostic laboratory system, wherein the second operation is one of the plurality of the operations used to perform the first test; (c) collectively analyzing the one or more first measurements and the one or more second measurements using a trained model with learned correlations between the first operation and the second operation; (d) determining an uncertainty score of the first test based on the collectively analyzing; and (e) determining whether to rerun the first test based on the uncertainty score.

[0005] In some embodiments, a method of determining accuracy of tests performed by a diagnostic laboratory system includes (a) generating a graphical representation of a workflow of a test performable by the diagnostic laboratory system, wherein the graphical representation comprises a plurality of nodes and is configured to be analyzed by a graph neural network; (b) obtaining one or more first measurements from a first operation performed by the diagnostic laboratory system during the test; (c) converting the one or more first measurements to a first vector, wherein the first vector is a first node of the graphical representation; (d) obtaining one or more second measurements from a second operation performed by the diagnostic laboratory system during the test; (e) converting the one or more second measurements to a second vector, wherein the second

vector is a second node of the graphical representation; (f) analyzing the first node and the second node using the graph neural network; (g) determining an uncertainty score of the test based on the analyzing; and (h) determining whether to rerun the test based on the uncertainty score.

[0006] In some embodiments, a diagnostic laboratory system includes one or more modules configured to perform a test, the test having a workflow of a sequence of operations; a plurality of sensors configured to generate one or more measurements for each of the operations; a processor coupled to the sensors; and a memory coupled to the processor. The memory includes a graph neural network and computer program code that, when executed by the processor, causes the processor to (a) generate a graphical representation of the workflow, wherein the graphical representation comprises at least a first node corresponding to a first operation of the workflow and a second node corresponding to a second operation of the workflow; (b) convert one or more first measurements resulting from the first operation to a first vector, wherein the first vector corresponds to the first node; (c) convert one or more second measurements resulting from the second operation to a second vector, wherein the second vector corresponds to the second node; (d) analyze the first vector and the second vector using the graph neural network; (e) determine an uncertainty score of the test based on analyzing the first vector and the second vector; and (f) determine whether to rerun the test based on the uncertainty score.

[0007] Still other aspects, features, and advantages of this disclosure may be readily apparent from the following description and illustration of a number of example embodiments, including the best mode contemplated for carrying out the disclosure. This disclosure may also be capable of other and different embodiments, and its several details may be modified in various respects, all without departing from the scope of the disclosure. This disclosure is intended to cover all modifications, equivalents, and alternatives falling within the scope of the claims and their equivalents.

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## Description

BRIEF DESCRIPTION OF THE DRAWINGS

[0008] The drawings, described below, are provided for illustrative purposes, and are not necessarily drawn to scale. Accordingly, the drawings and descriptions are to be regarded as illustrative in nature, and not as restrictive. The drawings are not intended to limit the scope of the disclosure in any way.

[0009] FIG. **1** illustrates a block diagram of a diagnostic laboratory system including a plurality of instruments according to one or more embodiments.

[0010] FIG. **2** illustrates a block diagram of an instrument of a diagnostic laboratory system showing modules and operations that may be performed by the instrument according to one or more embodiments.

[0011] FIG. **3** illustrates a block diagram of an aspiration and dispensing module that may be implemented in an instrument of a diagnostic laboratory system according to one or more embodiments.

[0012] FIG. **4** is a graph illustrating a pressure trace of a pipette assembly of an aspiration and dispense module located in a diagnostic laboratory system according to one or more embodiments.

[0013] FIG. **5**A illustrates an example method for determining an uncertainty score for a test of a diagnostic laboratory system and/or for determining whether to retest a sample according to one or more embodiments.

[0014] FIG. **5**B illustrates an example graph of a test workflow being processed by a graph neural network and an additional AI algorithm to produce an uncertainty score from a compact vector representation of operational data from operations performed during the test workflow, according to embodiments provided herein.

[0015] FIG. **5**C is a block diagram illustrating the use of algorithms to calculate an uncertainty

score resulting from testing of a sample by a diagnostic laboratory system according to one or more embodiments.
[0016] FIG. **6** illustrates a block diagram showing different sequences of operations that may be performed on samples during different tests performed by a diagnostic laboratory system according to one or more embodiments.
[0017] FIG. **7** illustrates a flowchart of a method of determining accuracy of tests performed by a laboratory system according to one or more embodiments.
[0018] FIG. **8** illustrates a flowchart of another method of determining accuracy of tests performed by a laboratory system according to one or more embodiments.

## DETAILED DESCRIPTION

[0019] Diagnostic laboratory systems conduct clinical chemistry and/or assays to identify analytes or other constituents in biological samples such as blood serum, blood plasma, urine, interstitial liquid, cerebrospinal liquids, and the like. The samples are collected in sample containers and transported to instruments and modules throughout the laboratory system where the samples are processed and analyzed. For example, the instruments and modules may prepare the samples for tests and conduct those tests on the samples.
[0020] When a sample is received in a diagnostic laboratory system for testing, the sample may go through a complex set of sequential operations of a workflow for each type of test. Different ones of the tests may require different sequences of operations. In some tests, the operations may commence with sample container handling where the sample container containing the sample is loaded into the laboratory system, for example. Sample container handling may include other operations such as reading labels on the sample container. Subsequent operations may include sample aspiration, reagent aspiration, and dispensing the sample and/or the reagent into a cuvette. A final operation in the sequence may include performing photometric measurements of a liquid in the cuvette to determine the concentration of a chemical or analyte in the sample. Other operations may be performed on the sample and/or the sample container. The operations may be performed using one or more instruments or modules configured to perform specific operations.
[0021] During each operation, a plurality of measurements may be performed. The measurements may include, for example, measurements of instrument performance, the sample, chemicals added to the sample, the sample container, position and/or pressure during an aspiration operation, and the like. A single operation may result in one or more measurements. In some embodiments, the instruments and/or modules of a diagnostic laboratory system may be configured to perform quality checks to validate the operations of the diagnostic laboratory system. These quality checks generate measurements of instrument performance.
[0022] The operations performed during testing are performed sequentially. In some instances, multiple minor errors, or measurements just within acceptable validity limits associated with individual operations, may accumulate and ultimately cause inaccurate test results. These inaccurate test results may include underestimated or overestimated analyte concentrations in the samples, which may cause unnecessary treatments to be prescribed to patients.
[0023] Unlike conventional laboratory systems, the diagnostic laboratory systems and methods disclosed herein collectively analyze a set of operations taken during laboratory tests and associate an uncertainty score (also referred to as a “biomarker confidence value”) with each laboratory test based on a cumulative effect of minor errors or measurements made during each operation within the sets. The uncertainty score or biomarker confidence value indicates whether an overall test result is valid or not. Thus, for clinical decisions, the uncertainty score can be used to determine whether test results can be relied on or whether retesting is required even though individual operational measurements may all be within acceptable limits. The uncertainty score may also indicate whether an instrument is failing. As described below, the uncertainty score or biomarker confidence value is not a simple average or median value based on validity scores of individual operation measurements.

[0024] As described previously, a test of a diagnostic laboratory system may include a plurality of sequential operations, and each operation may include a plurality of measurements. In some embodiments provided herein, a vector representation may be created for the measurements of each operation. For example, the vector representation may be an array of measurements which may be obtained by preprocessing raw measurement data (e.g., normalizing the data, mapping the data into a vector space using a dimensionality reduction technique such as principal component analysis (PCA) or independent component analysis (ICA), using an auto-encoder or other AI algorithm, or the like). The vector representation of each operation represents a “fingerprint” of the dynamics of the operation. Thereafter, the overall workflow of the test may be represented as a graph in which each node of the graph corresponds to a specific operation of the test. That is, each node of the graph is the vector representation (fingerprint) of the measurements of a different one of the test's operations.

[0025] A graph neural network may be trained to map the above-described workflow graph to a compact vector space representative of all the vector representation fingerprints of the test operations. For example, in some embodiments, a graph auto-encoder may be trained for this purpose. In one or more embodiments, the graph auto-encoder may include a graph encoder which maps all input operational data (e.g., the vector representation of each test operation) to the compact vector space, and a graph decoder, which reconstructs the operational data to its original form (e.g., for training purposes). The graph neural network may be trained on operation workflow data for the test obtained from the day-to-day operation of the diagnostic laboratory system. Such data may be collected from a deployed and fully operational diagnostic laboratory system, for example. Training may be performed continuously, periodically, or at any suitable time. Training may be performed while the diagnostic laboratory system is online (e.g., in use) or offline.

[0026] After obtaining the compact vector space representation of the operational data for the test, the compact vector space may be used with a neural network or other AI algorithm to estimate test uncertainty (e.g., via likelihood of test success from the graph-encoded vector representations of each test operation). Additionally, or alternatively, the compact vector space and neural network may be employed to determine an uncertainty score for each operation of the test. In some embodiments, the neural network (or other AI algorithm) used to determine test and/or operational uncertainties based on operational fingerprints (e.g., vector representations) of the test may be trained on data collected for failed operations or tests conducted in a controlled diagnostic laboratory or factory setting. Significantly, in such a controlled setting, a test in which each operation is within an acceptable range (e.g., passes a validity check for that operation) may be flagged as a failed test. For example, if all test operations individually produce valid results but several operations are close to failing, it may be desirable to re-run the test (e.g., if multiple operations are near an upper or lower validity limit for the operations, one operation is near an upper limit while another operation is near a lower limit, etc.). Thus, the neural network may be trained to provide uncertainty scores for tests and provide guidance as to whether a re-test is warranted regardless of whether individual operations within the test have passed or failed internal validity checks. Likewise, by being trained on numerous vector representations for individual operations within a test, the neural network may be trained to identify uncertainty scores for each operation within a test and/or whether to recommend a re-test based on an individual operation's uncertainty score (and/or any combination of individual operation uncertainty scores).

[0027] Example measurements may include pressure sensor measurements obtained during aspiration and dispensation of samples and reagents. Other measurements may include, for example, photometric, acoustic, temperature, and optical measurements. In some embodiments, the measurements may include results from quality check algorithms performed by instruments in the laboratory systems. Algorithms used herein may include, for example, deep neural networks, generative neural networks, graph neural networks, and other networks or AI algorithms.

[0028] These and other diagnostic laboratory systems and methods that determine accuracy or

uncertainty of tests are described in greater detail with reference to FIGS. **1**-**8**.

[0029] Reference is made to FIG. **1**, which illustrates a block diagram of an embodiment of a diagnostic laboratory system **100**. The diagnostic laboratory system **100** may include a plurality of instruments **102** configured to process samples and sample containers **104** (a few labelled) and to conduct tests (e.g., assays or other tests) on the samples. Performing the tests may include performing one or more operations on the samples. Each operation may include one or measurements. As described herein, one or more of the instruments **102** may include a plurality of different modules configured to perform the operations described herein. The samples may be various biological specimens collected from individuals, such as patients being evaluated by medical professionals. The samples may be collected in the sample containers **104** and delivered to the laboratory system **100** wherein the sample containers **104** can be transported by a track **108** throughout the laboratory system **100**. such as to different ones of the instruments **102**. Sample containers **104** may be transported by sample carriers **110** (a few labelled), for example. In the embodiment of FIG. **1**, the system **100** has three instruments **102**, which include a sample handler **114**, a first analyzer **116**, and a second analyzer **118**. The laboratory system **100** may include fewer or more instruments than shown in FIG. **1**.

[0030] In some embodiments, the track **108** may extend proximate or around the instruments **102** as shown in FIG. **1**. As described herein, portions or modules of the instruments **102** may have devices, such as robots (not shown in FIG. **1**), that transfer sample containers **104** to and from the sample carriers **110**. The track **108** may include a plurality of segments **120** (a few labelled) that may be interconnected. The sample carriers **110** may move as shown by the dashed lines **126** in the segments **120**. In some embodiments, some of the segments **120** may be integral with one or more of the instruments **102**.

[0031] Diagnostic laboratory systems, such as the laboratory system **100**, may have many instruments and may have tracks linked to other laboratory systems. The laboratory systems, including the laboratory system **100**, may simultaneously move and process a plurality of sample carriers **110** and their respective sample containers **104**. In some embodiments, the laboratory system **100** may move and process hundreds or thousands of sample carriers **110** and their respective sample containers **104** simultaneously.

[0032] The laboratory system **100** may include or be coupled to a computer **130** configured to execute one or more programs configured to control the laboratory system **100**. The computer **130** may be configured to communicate with the instruments **102** and other components of the laboratory system **100**, such as components in a transport system. The transport system may include some or all components configured to transport samples throughout the laboratory system **100** (e.g., motors, sensors, power supplies, etc.). The computer **130** may include a processor **132** configured to execute programs including programs other than those described herein. The programs may be implemented in computer code.

[0033] The computer **130** may include or have access to memory **134** that may store one or more programs and/or data. The memory **134** and/or programs stored therein may be referred to as a non-transitory computer-readable medium. The programs may be computer code executable on or by the processor **132**. The memory **134** may include an analysis program **136** configured to analyze operations performed by the instruments **102** and/or determine accuracy or uncertainty scores of tests performed by the instruments **102** as described herein. The analysis program **136** may include a plurality of different programs as described herein, including one or more AI algorithms (e.g., graph neural network **137**, other generative neural networks, other deep networks or AI algorithms including supervised, semi-supervised or unsupervised AI models, etc.). In some embodiments, the analysis program **136**, portions of the analysis program **136**, or copies of the analysis program **136** may reside in individual ones the instruments **102** or locations external to the diagnostic laboratory system **100**.

[0034] The computer **130** may be coupled to a workstation **138** that is configured to enable users to

interface with the laboratory system **100**. The workstation **138** may include a display **140**, a keyboard **142**, and other peripherals. The analysis program **136** or other programs may cause the display **140** to display results of data analysis including uncertainty scores (e.g., laboratory biomarker confidence values), test validity scores, and indications as to whether tests should be rerun. Thus, the computer **130** in conjunction with the workstation **138** may be configured to generate a notification of the accuracy of tests, such as uncertainty scores.

[0035] The analysis program **136** may perform many functions. In some embodiments, the analysis program **136** may operate in conjunction with other programs to perform the functions. For example, the analysis program **136** may be configured to detect operational failures in the laboratory system **100**. If any operation of the laboratory system **100** fails and goes undetected, the undetected failure can have a significant impact on clinical decision making. For example, the tests resulting from the failed operations may be inaccurate, which may cause medical professionals relying on the results to provide inaccurate remedies.

[0036] When a sample is received in the laboratory system **100** for testing, the sample undergoes a complex set of sequential operations or processes in a specific workflow that is defined by specific tests. Each type of test may have a unique sequence of operations. The workflow sequence may start with a sample handling or a sample container handling operation followed by operations of sample and/or reagent aspiration and dispensing into a cuvette. The mixture in the cuvette may undergo other operations required by the test. The workflow sequence may conclude with measurement operations, such as photometric measurements, to determine chemical properties of the sample.

[0037] Each of the operations in the workflow sequences may be performed using one or more of the instruments **102**. Because the operations occur sequentially, minor instrument errors and/or measurements within, but close to, acceptable limits associated with one or more of the operations may accumulate and result in larger errors in the resulting tests. In some embodiments diagnostic laboratory system **100** collectively analyzes the sequential sets of operations performed during tests and determines uncertainty scores of the test results performed within the laboratory system **100**. For example, each uncertainty score may be based on end-to-end validity checks of the operations or a set of the operations performed during a test to determine the accuracy of the test. In some embodiments, an uncertainty score may be used to determine if retesting may be required to obtain valid or more accurate test results.

[0038] Additional reference is made to FIG. **2**, which illustrates a block diagram of an instrument **202** showing modules and/or components associated with the instrument **202**, as well as operations associated therewith that may be performed by the instrument **202**. (Instrument **202** may be similar to one of the instruments **102** of FIG. **1**, for example.) In some embodiments, the modules and/or components of instrument **202** may be within the instrument **202** (e.g., not separate units occupying separate areas). In one or more embodiments, the instrument **202** may include a robot handler **210** that may be configured to grasp and move sample containers **104**, sample carriers **110**, and/or other containers (vials, cuvettes, and the like) within the instrument **202**. The robot handler **210** may operate with an internal transport system **212** that is configured to transport the sample containers **104**, the carriers **110**, and/or other containers via internal tracks to specific locations within the instrument **202**. The internal transport system **212** may be connected to track **108** of laboratory system **100** to receive and return the sample containers **104**, the carriers **110**, and/or other containers.

[0039] In some embodiments, the instrument **202** may include reagent storage **214**. The reagent storage **214** may be located in a module within the instrument **202** that is accessible by components of an aspiration and dispense module **216** that are configured to aspirate and dispense the reagents and the samples. A photometric analyzer **218** may perform photometric analysis on the samples with or without one or more reagents added to the samples. A quality check program **220** may perform self-checks and other analyses to determine whether the modules (e.g., modules **210**-**218**)

are performing correctly and/or a likelihood that operation results of instrument **202** are accurate. The quality check program **220** may operate with the analysis program **136** (FIG. **1**) and/or transmit quality check measurements to the analysis program **136**.

[0040] Additional reference is made to FIG. **3**, which illustrates a block diagram of an embodiment of the aspiration and dispense module **216**. The aspiration and dispense module **216** may be implemented in one or more of the instruments **102** (FIG. **1**) or the instrument **202** (FIG. **2**). Other embodiments of the aspiration and dispense module **216** may be used in the instruments **102** and/or the instrument **202**. The embodiment of FIG. **3** illustrates a sample container **304** located in a carrier **310**, which is illustrative of the sample containers **104** and the carriers **110** (FIG. **1**). The carrier **310** may have been transported to the aspiration and dispense module **216** by the internal transport system **212** (FIG. **2**). The sample container **304** may contain a sample **306** that is to be analyzed, processed, and/or tested by the instrument **202** and/or other ones of the instruments **102** (FIG. **1**).

[0041] The aspiration and dispense module **216** may include reagents **312** stored in a reagent pack **314**. As described in greater detail herein, components of the aspiration and dispense module **216** may aspirate the reagents **312** from the reagent pack **314** and the sample **306** from the sample container **304**. In some embodiments, the aspiration and dispense module **216** may include a tip dispenser **316** configured to change aspiration probe tips as described herein prior to aspiration operations. The aspiration and dispense module **216** may have a cuvette **320** configured to receive aspirated portions of the reagents **312** and the sample **306** via dispense operations. In some embodiments, the contents of the cuvette **320** may undergo photometric analysis performed by the photometric analyzer **218** (FIG. **2**).

[0042] The aspiration and dispense module **216** may include a robot **331** that is configured to move a pipette assembly **332** within the aspiration and dispense module **216**. In the embodiment of FIG. **3**, a probe **334** of the pipette assembly **332** is shown preparing to aspirate a reagent **312** from the reagent pack **314**. The probe **334** is shown with a tip **322** attached to an end of the probe **334**. The tip **322** may have been placed on the probe **334**, such as by the tip dispenser **316** prior to aspirating the reagents **312**. A new tip may be placed on the probe **334** by a tip replacement operation, such as by use of the tip dispenser **316** prior to aspirating the reagent **312** or the sample **306**.

[0043] The sample container **304** is shown in FIG. **3** without a cap, which may have been removed by a decapping module (not shown) in the instrument **202** or by another module (not shown) in the laboratory system **100** that performs a decapping operation. Removal of the cap enables the sample **306** to be aspirated. The pipette assembly **332** may be configured to position the probe **334**, by use of the robot **331**, to aspirate and dispense the reagents **312** and the sample **306**. The reagents **312**, other reagents, and a portion of the sample **306** may be dispensed into a reaction vessel, such as the cuvette **320** by moving the probe **334** to an appropriate location and performing a dispense operation. The cuvette **320** may be made of a material that passes light for photometric analysis by the photometric analyzer **218** (FIG. **2**) as described herein.

[0044] Some components of the aspiration and dispense module **216** may be electrically coupled to a computer **330**. In the embodiment of FIG. **3**, the computer **330** may include a processor **330**A and memory **330**B. Programs **330**C may be stored in the memory **330**B and may be executed by the processor **330**A. In other embodiments, the computer **330** and/or components of the computer **330** may be implemented in the computer **130** (FIG. **1**). One of the programs **330**C may be the quality check program **220** (FIG. **2**). The computer **330** may also include an aspiration/dispense controller **330**D and a position controller **330**E that may be controlled by programs, such as the programs **330**C stored in the memory **330**B. In some embodiments, the position controller **330**E and/or the aspiration/dispense controller **330**D may be implemented in separate devices (e.g., other computers). The programs **330**C may include algorithms that control and/or monitor components within the aspiration and dispense module **216**. In some embodiments, the algorithms may include the position controller **330**E and/or the aspiration/dispense controller **330**D.

[0045] The robot **331** may include one or more arms and motors that are configured to move the pipette assembly **332** within the aspiration and dispense module **216**. In the embodiment of FIG. **3**, the robot **331** may include an arm **350** coupled between a first motor **352** and the pipette assembly **332**. The first motor **352** may be electrically coupled to the computer **330** and may receive instructions generated by the position controller **330**E. The instructions may instruct the first motor **352** to move in specific directions and speeds. The first motor **352** may be configured to move the arm **350** to enable the probe **334** to aspirate and/or dispense the sample **306** and/or reagents **312** as described herein. The first motor **352** may include or be associated with a position sensor **352**A that is configured to generate measurements (e.g., sensor data) indicating the position of the arm **350**. Measurement data generated by the position sensor **352**A may be transmitted to the computer **330** and/or the computer **130** (FIG. **1**) and may be used by the analysis program **136** as described herein.
[0046] A second motor **354** may be coupled between the arm **350** and the pipette assembly **332** and may be configured to move the probe **334** in a vertical direction (e.g., a Z-direction) to aspirate and/or dispense liquids as described herein and to replace the tip **322**. The second motor **354** may move the probe **334** in response to instructions generated by the programs **330**C. For example, the second motor **354** may enable the probe **334** to enter into and recede from the sample container **304**, the cuvette **320**, the tip dispenser **316**, and/or the reagent pack **314**. The second motor **354** may include or be associated with a current sensor **354**A that is configured to measure current drawn by the second motor **354**. Measurements or sensor data (e.g., measured current) generated by the current sensor **354**A may be transmitted to the computer **330** and/or the computer **130** (FIG. **1**) and may be used by the analysis program **136** as described herein.
[0047] The aspiration and dispense module **216** may include a plurality of position sensors configured to generate measurements related to the positions of components. In the embodiment of FIG. **3**, a position sensor **356** may be mechanically coupled to the robot **331**. In some embodiments, the position sensor **356** may be coupled to other components in the aspiration and dispense module **216**. The position sensor **356** may be configured to sense positions of one or more components of the robot **331** or other components within the aspiration and dispense module **216**, such as the pipette assembly **332**. In the embodiment of FIG. **3**, the position sensor **356** may measure the position of the arm **350**, the pipette assembly **332**, and/or the probe **334**. The measurements (e.g., position data) may be transmitted to the computer **330** and/or the computer **130** for processing by the analysis program **136** as described herein.
[0048] The aspiration and dispense module **216** may also include a pump **360** mechanically coupled to a conduit **362** and electrically coupled to the aspiration/dispense controller **330**D. The pump **360** may generate a vacuum or negative pressure (e.g., aspiration pressure) in the conduit **362** during aspiration operations. The pump **360** may generate a positive pressure (e.g., dispense pressure) in the conduit **362** during dispense operations.
[0049] A pressure sensor **364** may be configured to measure pressure in the conduit **362** and generate measurements (e.g., pressure data) indicative of the pressure. In some embodiments, the pressure sensor **364** may be configured to measure aspiration pressure and generate pressure measurements. In some embodiments, the pressure sensor **364** may be configured to measure dispense pressure and generate pressure measurements. For example, the pressure measurements may be in the form of a pressure trace as a function of time and as described with reference to FIG. **4** below. The pressure measurements ultimately may be transmitted to the computer **130** (FIG. **1**) and/or the computer **330** for processing by the analysis program **136**. The pressure traces may change as a function of time or when one or more components of the aspiration and dispense module **216** are replaced or failing.
[0050] Additional reference is made to FIG. **4**, which is a graph illustrating an example of a pressure trace **400** of the pipette assembly **332** measured by the pressure sensor **364** as a function of time. In the embodiment of FIG. **4**, the pressure trace **400** shows pressure in the pipette assembly

**332** during tip pickup, aspiration, and dispense operations. The pressure rises slightly as the tip **322** is replaced and dips significantly during the aspiration process. The pressure then rises significantly during the dispense operation. The pressure trace **400** represents one or more measurements that may be analyzed by the analysis program **136** as described herein.

[0051] Referring again to FIG. **3**, the aspiration and dispense module **216** may include an imaging device **366** configured to capture images of the probe **334** and/or liquids in the probe **334**. For example, the probe **334** may be transparent so the imaging device **366** can capture images of liquids located in the probe **334**. The captured images may comprise image data that is transmitted to and analyzed by the computer **330** and/or the computer **130** (FIG. **1**) for processing by the analysis program **136**. The image data may include measurements generated during imaging operations, such as during photometric analysis. The programs **330**C (or the analysis program **136** of FIG. **1**) may analyze the image data to determine the quality of the liquid in the probe **334**. For example, the programs **330**C or the analysis program **136** may determine whether the liquid in the probe **334** contains bubbles or other anomalies.

[0052] As described herein, one or more modules or components, such as aspiration and dispense module **216**, of an instrument may include one or more sensors that may be monitored by one or more programs such as programs **330**C. Example sensors include position sensors, pressure sensors, imaging sensors, etc. Programs such as programs **330**C also may perform quality check (e.g., self-test) routines on the sensors. This information may be provided to computer **130** and/or analysis program **136** (FIG. **1**). As described further below, data generated by the self-test routines and sensors include measurements that may be encoded to vector space and/or analyzed by one or more AI algorithms, such as by computer program code in the analysis program **136** (FIG. **1**), For example, a first AI algorithm may generate a fingerprint of the dynamics of each operation of a test via a vector representation of operational data (e.g., sensor measurements, self-test measurements, etc.) while a second AI algorithm may analyze the vectors (e.g., the fingerprints) of the various operations of the test to determine the accuracy of the test, such as by calculating or otherwise determining an uncertainty score (e.g., a biometric confidence value).

[0053] In greater detail, the analysis program **136** may employ AI algorithms to analyze collective operational data generated by the instruments **102**. Based on the analysis, the analysis program **136** may calculate an uncertainty score (e.g., a biomarker confidence value) that is an indication of the validity or accuracy of a test performed on a sample such as sample **306**. In some embodiments, the instrument measurements may include, but are not limited to, the pressure sensor measurements obtained during aspiration and dispensation of sample and reagents, such as shown by the pressure trace **400** (FIG. **4**). Other measurements may include position data, image data, photometric measurements, acoustic measurements, temperature measurements, optical measurement, quality check or self-check measurements, or the like.

[0054] In some embodiments, measurements obtained during each operation of a test are encoded as specific fingerprints (e.g., vectors) representative of the dynamics of the operations. A first AI algorithm trained with learned correlations between operations, such as learned correlations such as between a first operation and a second operation, may then map the fingerprint vector representations to a compact vector space. One or more other AI algorithms are configured to collectively analyze the compact vector space to determine the accuracy of the test, such as by calculating the uncertainty score. In some embodiments, if the uncertainty score is below a predetermined value, the computer **130** (FIG. **1**) may generate a notification that the test is not valid and/or that a retest may be required.

[0055] FIG. **5**A illustrates an example method **500** for determining an uncertainty score for a test of a diagnostic laboratory system and/or for determining whether to retest a sample in accordance with one or more embodiments. FIG. **5**B illustrates an example graph **502** of a test workflow being processed by a graph neural network **504** and an additional AI algorithm (e.g., neural network **506**) that produces an uncertainty score **508** from a compact vector representation **510** of operational

data from operations (e.g., operations O**1**-O**6**) performed during the test workflow, in accordance with embodiments provided herein.

[0056] With reference to FIG. **5**A, in block **512**, measurements are obtained for each operation within a test. For example, pressure, temperature, photometric, acoustic, or other parameters, self-test or quality-check measurements, etc., for each operation of a test may be obtained (e.g., provided to computer **130** and/or analysis program **136**). Example operations include sample container handling operations, sample aspiration and dispense, reagent aspiration and dispense, photometric measurements to determine chemical concentration and/or assay type, and/or any other test operations.

[0057] In block **514**, a vector representation may be created for the measurements of each test operation. For example, a vector representation may be an array of measurements which may be obtained by preprocessing raw measurement data (e.g., normalizing the data, mapping the data into a vector space using a dimensionality reduction technique such as principal component analysis (PCA) or independent component analysis (ICA), using an auto-encoder or other AI algorithm, or the like). The vector representation of each operation represents a “fingerprint” of the dynamics of the operation.

[0058] Thereafter, in block **516**, a graph of workflow for the test may be created. Specifically, the overall workflow of the test may be represented as a graph in which each node of the graph corresponds to a specific operation of the test. That is, each node of the graph is the vector representation (fingerprint) of the measurements of a different one of the test's operations. For example, graph **502** of FIG. **5**B illustrates an example test workflow with six operations (labelled O**1**-O**6**). Other numbers and/or order of operations may be used. Measurements made during each operation O**1**-O**6** are encoded in a vector representation that corresponds to a node (e.g., nodes N**1**-N**6**, respectively) of graph **502** (see also FIG. **6** described below).

[0059] In block **518**, a graph neural network is used to map the workflow graph into a compact vector space. For example, a graph neural network may be trained to map a test workflow graph to a compact vector space representative of all the vector representation fingerprints of the test operations. In FIG. **5**B, graph neural network **504** has been trained to map workflow graph **502** to compact vector space **510**. In some embodiments, a graph auto-encoder may be trained for this purpose. In one or more embodiments, the graph auto-encoder may include a graph encoder which maps all input operational data (e.g., the vector representation of each test operation) to the compact vector space, and a graph decoder, which reconstructs the operational data to its original form (e.g., for training purposes). In FIG. **5**B, a graph encoder **517** maps graph **502** to compact vector space **510** and graph decoder **517**′ reconstructs graph **502** (as graph **502**′). The graph neural network may be trained on operation workflow data for the test, for example, operation workflow data obtained from the day-to-day operation of the diagnostic laboratory system. Such data may be collected from a deployed and fully operational diagnostic laboratory system, for example. Training may be performed continuously. periodically, or at any suitable time. Training may be performed while the diagnostic laboratory system is online (e.g., in use) or offline.

[0060] After obtaining the compact vector space representation of the operational data for the test, in block **520**, the compact vector space may be used with a neural network or other AI algorithm to estimate test uncertainty (e.g., compute an uncertainty score for the test, such as likelihood of test success, from the graph-encoded vector representations of each test operation). Additionally, or alternatively, in block **522**, the compact vector space and neural network (or other AI algorithm) may be employed to determine an uncertainty score for each operation of the test. For example, in FIG. **5**B, neural network **506** may be trained for this purpose. In some embodiments, the neural network (or other AI algorithm) used to determine test and/or operational uncertainties based on operational fingerprints (e.g., vector representations) of the test may be trained on data collected for failed operations or tests conducted in a controlled diagnostic laboratory or factory setting. Significantly, in such a controlled setting, a test in which each operation is within an acceptable

range (e.g., passes a validity check for that operation) may be flagged as a failed test. For example, if all test operations individually produce valid results but several operations are close to failing, it may be desirable to re-run the test (e.g., if multiple operations are near an upper or lower validity limit for the operations, one operation is near an upper limit while another operation is near lower limit, etc.). Thus, the neural network may be trained to provide uncertainty scores for tests and provide guidance as to whether a re-test is warranted regardless of whether individual operations within the test have passed or failed internal validity checks. Likewise, by being trained on numerous vector representations for individual operations within a test, the neural network may be trained to identify uncertainty scores for each operation within a test and/or whether to recommend a re-test based on an individual operation's uncertainty score (and/or any combination of individual operation uncertainty scores).

[0061] Any suitable neural networks may be employed. Example architectures include Inception, ResNet, ResNeXt, DenseNet, or the like, although other CNN architectures may be employed.

[0062] In block **524**, based on an uncertainty score for the overall test workflow and/or based on one or more uncertainty scores for individual operations, a determination as to whether to retest may be made and/or provided to a user. In some embodiments, method **500**, graph neural network **504**, and/or neural network **506** may be implemented in computer **130**, memory **134**, and/or analysis program **136** (e.g., as computer program code), and analysis program **136** may make retest recommendations and/or execute retesting.

[0063] As stated, in some embodiments, neural network **506** (or another AI algorithm) used to determine test and/or operational uncertainties based on fingerprints (e.g., vector representations) of test operations may be trained on data collected for failed operations or tests conducted in a controlled diagnostic laboratory or factory setting. For example, in a controlled diagnostic laboratory, it may be determined that a creatinine concentration test may produce a creatinine concentration value with a variance of +/−0.1 mg/dL under some conditions. Neural network **506** may be trained to provide the estimated creatinine concentration variance, and in some embodiments, recommend a re-test based on the variance. For instance, if a test produces a creatinine concentration value of 0.5 mg/dL+/−0.1 mg/dL, neural network **506** may recommend that for such a low value, the creatinine concentration should be re-tested even though each operation of the creatinine concentration test produced measurements within a valid range (and/or each operation passed its own internal self-check or quality check). Additionally, or alternatively, neural network **506** may be trained to produce an uncertainty score that represents a confidence level, such as 50%, 70%, 90%, or the like, based on operational fingerprints of a test. In some embodiments, a creatinine concentration value of a 0.5 mg/dL with 50% confidence may be flagged for retest even though each operation of the creatinine concentration test produced measurements within a valid range.

[0064] In another example embodiment, a test may include obtaining a first measurement during a first operation of the test, wherein the first measurement has a value below, but near, an upper first measurement validity limit. For example, the first measurement may be an aspiration pressure of a reagent that is below, but near an upper validity limit. The test may further include obtaining a second measurement during a second operation of the test, wherein the second measurement has a value above, but near, a lower second measurement validity limit. For example, the second measurement may be an aspiration pressure of a sample that is above, but near a lower validity limit. Detailed analysis in a controlled or factory setting may indicate that, in such cases, a re-test is recommended. The neural network **506** may be trained to provide a low (e.g., failing) uncertainty score in such instances. Specifically, the first and second measurements may be collectively analyzed using a trained model (e.g., neural network **506**) with learned correlations between the first operation and the second operation and the neural network **506** may provide a failing uncertainty score for the test based on the collectively analyzing.

[0065] A neural network or other AI algorithm (e.g., neural network **506**) may be trained to

determine if an individual operation has succeeded or failed, and/or, in some embodiments, to provide an uncertainty score for the individual operation. In one embodiment, for example, an uncertainty score for an individual operation may be obtained by training an ensemble of neural networks wherein each network is trained to provide a “likelihood” of whether the operation succeeded. Given a set of likelihoods from the ensemble of networks, a final decision as to whether the operation succeeded or failed may be based on the majority or the mean likelihood score. In addition, the variance of the likelihoods from the ensemble of networks may be used to estimate the uncertainty (and/or uncertainty score) of the individual operation. If the variance is high, this implies the networks in the ensemble do not agree on whether the operation succeeded and hence the uncertainty (and uncertainty score) would be high, and vice versa. As an example, an ensemble of three neural network models may be used to evaluate the same operation. In some embodiments, the neural networks may be different types of networks and/or differently trained neural networks. Assume that network models 1, 2 and 3 output the likelihood of success as 1, 0.8, and 0.1 respectively (with 1 being a high likelihood of success). Using a majority approach, the operational would be reported as having succeeded. However, the uncertainty score of the assessment is high because variance is high (e.g., a standard deviation of 0.47). If the same network ensemble outputs were 1.0, 0.8, and 0.9, then the uncertainty score would be low (e.g., standard deviation of 0.1). In another embodiment, a neural network may output a likelihood of success (or uncertainty score) that is proportional to the confidence of the network. For example, a neural network with a Gaussian process classification layer may be used (see, for example, Amersfoort et al., “On Feature Collapse and Deep Kernel Learning for Single Forward Pass Uncertainty,” Arxiv, arXiv.2102.11409, 22 Feb. 2021, https://arxiv.org/abs/2102.11409). In yet another embodiment, an output of a neural network may be explicitly calibrated to be proportional to confidence (e.g., outputting a likelihood of success and/or an uncertainty score for an individual process) such as by using a Platt Calibration or similar algorithm.

[0066] Thus, a neural network or other AI algorithm may be trained to provide uncertainty scores for tests and provide guidance as to whether a re-test is warranted regardless of whether individual operations within the test have passed or failed internal validity checks. Likewise, by being trained on numerous vector representations for individual operations within a test, the neural network may be trained to identify uncertainty scores for each operation within a test and/or whether to recommend a re-test based on an individual operation's uncertainty score (and/or any combination of individual operation uncertainty scores).

[0067] Additional reference is made to FIG. **1** and FIG. **5**C, which is a block diagram **520** illustrating the use of AI algorithms to calculate an uncertainty score **545** according to one or more embodiments. In the embodiment of FIG. **5**C, several operations **530** or procedures may be used by the diagnostic laboratory system **100** to test the sample **306** (FIG. **3**). Measurements from each of the operations **530** may be encoded as specific fingerprints or vectors representative of the individual operations. In the embodiment of FIG. **5**C, the operations **530** include sample handling **532**, sample aspiration **534**, reagent aspiration **536**, and photometric analysis **538**. The laboratory system **100** may perform other operations. Each of the operations **530** may be performed in one or more of the instruments **102**. Measurements, such as test measurements and measurements generated by self-test programs, may be received in operational block **540**.

[0068] The measurements generated by the sample handling **532** may be in the form of system logs that record actions performed during the sample handling and any anomalies occurring during the sample handling **532**. The measurements generated by the sample handling **532** may be in other forms. For example, the measurements may include pressure applied to grippers to grasp the sample containers **104**, weight of the sample containers **104**, identification information in the form of image data, and other measurements.

[0069] The sample aspiration **534** and reagent aspiration **536** may generate measurements or data as described with regard to the aspiration and dispense module **216** of FIG. **3**. The measurements

may include pressure traces as illustrated by the pressure trace **400** in FIG. **4** and sensor measurements from the sensors. The measurements may be related to other operations, such as image data indicating whether aspirated liquids contain bubbles. The photometric analysis **538** may generate signal traces or other types of measurements or data commonly generated by photometric analyzers.

[0070] The measurements from operational block **540** may be received in operational block **542** where the specific fingerprints representative of the dynamics of the operations **530** are generated. The fingerprints may be encoded into vectors, such as compact vectors. The vector representations may be arrays of measurements obtained by preprocessing raw data generated by one or more of the instruments **102** (FIG. **1**) during performance of the operations **601**. In some embodiments, preprocessing may involve normalizing the data over a collection of measurements over a feasible or predetermined range of measurements. In other embodiments, preprocessing may involve projection of the raw data to a vector space using dimensionality reduction techniques such as principal component analysis (PCA), independent principal component analysis (ICA), or auto-encoders.

[0071] In some embodiments, AI, such as deep networks, generative neural networks, and other trained models may be used to generate the vectors. In some embodiments, each of the vectors may represent an individual operational validity score of the measurements received from operations **530**.

[0072] The vectors generated by the operational block **542** may be analyzed by one or more AI algorithms in operational block **544** to determine the accuracy of the tests. For example, the one or more AI algorithms in operational block **544** may generate the uncertainty score. In some embodiments, the operational block **544** may use a graph neural network (GNN) plus an additional AI algorithm (e.g., a neural network) to calculate the uncertainty score as described previously with references to FIGS. **5**A and **5**B. Accordingly, the one or more AI algorithms can learn a combined representation of heterogeneous data or measurements from the modules and/or operations and estimate a confidence score associated with the tests. The methods described herein, such as through the analysis program **136**, can be applied to determine the uncertainty score (e.g., accuracy) of the entire set of operations performed during a laboratory test.

[0073] The process described in FIG. **5**C may be applied to a sample test that includes operations described with reference to FIGS. **3** and **4** to analyze aspiration and dispensing operations in addition to other operations. Because an invalid operation, such as an invalid aspiration operation, increases the likelihood that the subsequent dispensing operation will be invalid and increases the uncertainty of the test. the joint analysis is better equipped to generate an accurate uncertainty score than analyzing each operation individually. Another example relates to the sample and reagent volumes used in the test. For example, the volume of the aspirated sample may be lower than expected but within predetermined limits and the volumes of the aspirated reagents may be greater than expected but within predetermined limits. When analyzed individually, the test would indicate a high likelihood of being valid. However, even though the individual volumes are within their respective predetermined limits, the analyte concentration calculated by the test may not be accurate. Thus, for example, an uncertainty score may be calculated that is less than a predetermined value, which indicates that the associated test should be rerun. In some embodiments, an uncertainty score below a predetermined value may cause computer **130** (executing analysis program **136**) to automatically reschedule the associated test.

[0074] Other testing procedures and descriptions using graph neural networks (GNNs) will now be described. Referring to the instrument **202** of FIG. **2**, the instrument **202** may be configured to perform a plurality of different tests. For example, some tests may be performed using reagents and some tests may be performed without using reagents. Additional reference is made to FIG. **6**, which illustrates a block diagram **600** (also referred to as graph **600**) showing different sequences of operations **601** that may be performed on samples to conduct different tests or different types of

tests according to one or more embodiments. Different instruments may perform different ones of the operations **601** and may perform different sequences of the operations **601** depending on the tests being conducted. The sequences of the operations **601** for individual tests may be referred to as individual workflows. Thus, the block diagram **600** illustrates graphical representations of the workflows.

[0075] One or more of the operations **601** may be a node of a graph of a test workflow (e.g., graph **600** or graph **502** of FIG. **5**B) and paths between the operations **601** may be edges of the graph. Each of the operations **601** may generate measurements that may be encoded to the vectors or compact vectors (e.g., reduced dimension vectors) as described previously. A GNN may map the vector representation fingerprints to a compact vector space (e.g., compact vector space **510**) and another AI algorithm (e.g., neural network **506**) may collectively analyze the measurements (via fingerprint vector representations) to determine the accuracy (e.g., uncertainty score) of the test.

[0076] The diagram **600** shows the workflows, including operational sequences, for different tests that the instrument **202** may perform. For example, a first operation may be tip pickup **602** wherein the probe **334** (FIG. **3**) may replace a tip (e.g., tip **322**—FIG. **3**) prior to aspirating a sample or a reagent. The tip pickup **602** may include moving the probe **334** to the tip dispenser **316** and replacing the tip **322**. After the tip pickup **602**, processing may proceed to either sample aspiration **604** or reagent aspiration **606**. If a reagent is not to be added to the sample, e.g., processing may proceed directly to sample aspiration **604**. The path from the sample aspiration **604** may extend to sample dispense **608** and the path from reagent aspiration **606** may extend to reagent dispense **610**. In some embodiments, the sample aspiration **604** and the sample dispense **608** may be a single operation or single node of a graph. In some embodiments, the reagent aspiration **606** and the reagent dispense **610** may be a single operation or single node of a graph. Paths from both the sample dispense **608** and the reagent dispense **610** may extend to the photometric analysis **612**. A path from the reagent dispense **610** may extend back to the tip pickup **602** prior to adding new liquids, such as new reagents, to the cuvette **320**. Other embodiments of the diagram **600** may include different paths depending on the configuration of the instruments and the tests that the instruments are configured to perform.

[0077] Different tests or different types of tests may have different workflows, such as different paths or edges from start to finish. For example, a first test having a first workflow may commence with tip pickup **602** followed by sample aspiration **604**. After sample aspiration **604**, the test may proceed with sample dispense **608** followed by photometric analysis **612**. A second test may have a second workflow and may commence with tip pickup **602**, followed by sample aspiration **604**. After sample aspiration **604**, the test may continue with sample dispense **608** followed by tip pickup **602** to receive a new tip (e.g., tip **322**—FIG. **3**) on the probe **334** (FIG. **3**). The test may proceed to reagent aspiration **606**, reagent dispense **610**, and may terminate with photometric analysis **612**. A third test may have a third workflow and commence with tip pickup **602**, followed by sample aspiration **604**. After sample aspiration **604**, the test may continue to sample dispense **608** followed by tip pickup **602** to receive a new tip on the probe **334**. The test may proceed to reagent aspiration **606**, then reagent dispense **610**, and back to the tip pickup **602**. When a new tip is received on the probe **334**, the test may proceed to reagent aspiration **606** and reagent dispense **610** to add new reagents to the cuvette **320**. This loop may continue to add new reagents to the cuvette **320**. The test may then terminate with photometric analysis **612**.

[0078] Measurements from each of the operations **601** may be encoded into vectors as described with regard to operational block **542** (FIG. **5**C). The nodes in the diagram (graph) **600** may then be analyzed by a GNN and then by an additional AI algorithm, such as described with regard to operational block **544** (FIG. **5**C). In some embodiments, the AI algorithm may be a neural network. The workflows (e.g., paths or edges) for each of the tests may be analyzed, such as was described with regard to calculating the uncertainty score **545** (FIG. **5**C). The AI algorithm may also generate the uncertainty score **545** as described herein.

[0079] In more detail, in some embodiments, the analysis program **136** may obtain measurements for individual ones of the operations **601** that collectively perform a test. The analysis program **136** may encode the measurements generated during each of the operations **601** into vector representations. For example, the vector representations may be arrays of measurements obtained by preprocessing raw data generated by one or more of the instruments **102** (FIG. **1**) during performance of the operations **601**. In some embodiments, preprocessing may involve normalizing the data over a collection of measurements over a feasible or predetermined range of measurements. In other embodiments, preprocessing may involve projection of the raw data to a vector space using dimensionality reduction techniques such as principal component analysis (PCA), independent principal component analysis (ICA), or auto-encoders.
[0080] The analysis program **136** may then use GNNs and/or other neural networks to learn operational manifolds of the instruments **102** and/or the laboratory system **100**. The operation manifolds may be workflows for different tests as described herein. An autoencoder, such as a variational graph autoencoder (which may include a graph decoder), or other algorithm may be trained to map all the input operational data (e.g., the measurements obtained during testing) to a compact vector space or other vector space. A graph decoder or other decoder may be trained to reconstruct the operational data from the compact vector space or other space (for training purposes). In some embodiments, the model that includes the encoders, decoders, and/or neural networks, may be trained over a large cohort of the operational workflow data and/or measurements obtained from day-to-day operations of the laboratory system **100** (FIG. **1**). The edges (paths) of the diagram (graph) **600** may be directed to represent the order or sequence in which the operations are performed for each type of test. The sequences thus model the causal structure of the workflow used to perform the tests. The above-described processes may be implemented in AI algorithms in the analysis program **136** and may enable the projection of operational workflow data to a vector representation.
[0081] The model(s) implemented in the analysis program **136** may then be used to detect operational anomalies or recognize operational failures in specific tests. Detection of operational anomalies may be performed by using a compact vector space generated by the trained GNN and constrained to be a Gaussian or a mixture-of-Gaussian distribution. Operational instances that project further away, such as using Mahalanobis distance, may be considered anomalous and may be attributed to operational anomalies. The Mahalanobis distance is a multivariate distance metric that measures the distance between a point and a distribution.
[0082] Training of the AI algorithm that generates an uncertainty score from a GNN generated compact vector space may be conducted in controlled laboratories or factory settings where data corresponding to failed operations and/or tests can be obtained. This data can then be combined with a large cohort of data corresponding to successful operations and/or tests to train a neural network to estimate the likelihood of operational success from a graph encoded vector representation used in the GNN. Together with the calculated likelihood score, the neural network may also estimate a validity score associated with each operation that correlates with the operation being the source of a high uncertainty or low uncertainty score. Equipped with such training, the analysis program **136** or other programs may recommend a retest or a user can determine if a retest may be necessary based on the uncertainty score. The status of operations may also be logged in machine logs, such as logs stored in the memory **134** (FIG. **1**) and can be used to determine if a specific operation is resulting in consistently low uncertainty scores and whether the corresponding module needs to be revised, serviced, or replaced.
[0083] An example of the methods and apparatus disclosed herein may be illustrated by a test performed by at least one of the instruments **102** that includes one reagent added to a sample followed by photometric analysis. Referring to FIG. **6**, the workflow for the test has the following sequence: tip pickup **602**, sample aspiration **604**, sample dispense **608**, tip pickup **602**, reagent aspiration **606**, reagent dispense **610**, and photometric analysis **612**. Measurements are obtained

during each of the operations in the workflow. For example, during tip pickup **602**, the measurements may include the pressure measurement (trace) shown in FIG. **4** and position sensor measurements generated by the position sensor **352**A and the position sensor **356**. These measurements may be encoded into a vector. Measurements generated by other ones of the operations in the workflow may also be encoded into vectors. In some embodiments, the operational block **542** may generate the vectors. A generative adversarial network (GAN), a GNN or other network or model trained on the test workflow may analyze the vectors to generate a compact vector space representation of operational fingerprints of the test that is analyzed by another AI algorithm (e.g., neural network **506**) to determine the uncertainty score **545**. Based on the uncertainty score **545**, the computer **130** may suggest a retest or indicate that the test is valid. For example, the information regarding the uncertainty score **545** may be output to the display **140**.

[0084] Reference is now made to FIG. **7**, which is a flowchart illustrating a method **700** of determining accuracy of tests performed by a laboratory system (e.g., laboratory system **100**) according to one or more embodiments. The method **700** includes, at block **702**, obtaining one or more first measurements during a first operation performed by the laboratory system, wherein the first operation is one of a plurality of operations used to perform a first test on a sample (e.g., sample **306**). The method **700** includes, at block **704**, obtaining one or more second measurements during a second operation performed by the laboratory system, wherein the second operation is one of the plurality of the operations used to perform the first test. The method **700** includes, at block **706**, collectively analyzing the one or more first measurements and the one or more second measurements using a trained model based on learned correlations between the first operation and the second operation (e.g., graph neural network **504** and/or neural network **506**). The method **700** includes, at block **708**, calculating an uncertainty score of the first test based on the analyzing. And the method **700** includes, at block **710**, determining whether to rerun the first test based on the uncertainty score. For example, analysis program **136** may alert a user to re-run the first test. Method **700** may optionally include rerunning the first test in response to the determination made at block **710**, such as when the calculated uncertainty score is less than a predetermined value. In some embodiments, the laboratory system **100** (e.g., computer **130** executing analysis program **136**) may automatically initiate the rerunning of the first test.

[0085] Reference is now made to FIG. **8**, which is a flowchart illustrating a method **800** of determining accuracy of tests performed by a laboratory system (e.g., laboratory system **100**) according to one or more embodiments. The method **800** includes, at block **802**, generating a graphical representation of a workflow of a test performable by the laboratory system, wherein the graphical representation comprises a plurality of nodes and is configured to be analyzed by a graph neural network (see, for example, test workflow graph **502** of FIG. **5**A or test workflow graph **600** of FIG. **6**). The method **800** includes, at block **804**, obtaining one or more first measurements from a first operation performed by the laboratory system during a test. The method **800** includes, in block **806** converting the one or more first measurements to a first vector, wherein the first vector is a first node of the graphical representation. The method **800** includes, in block **808**, obtaining one or more second measurements from a second operation performed by the laboratory system during the test. The method **800** includes, in block **810**, converting the one or more second measurements to a second vector, wherein the second vector is a second node of the graphical representation. The method **800** includes, in block **812**, collectively analyzing the first node and the second node using the graph neural network. For example, graph neural network **504** may generate a compact vector space representation of the graphical representation (e.g., graph **502** or **600**). The method **800** includes, in block **814**, determining an uncertainty score of the test based on the analyzing. As described, in some embodiments, the compact vector space may be fed to a trained neural network (e.g., neural network **506**) to determine the uncertainty score for the test. The method **800** includes, at block **816**, determining whether to rerun the test based on the uncertainty score.

[0086] While the disclosure is susceptible to various modifications and alternative forms, specific

method and apparatus embodiments have been shown by way of example in the drawings and are described in detail herein. It should be understood, however, that the particular methods and apparatus disclosed herein are not intended to limit the disclosure but, to the contrary, to cover all modifications, equivalents, and alternatives falling within the scope of the claims.

## Claims

**1**. A method of determining accuracy of tests performed by a diagnostic laboratory system, comprising: obtaining one or more first measurements during a first operation performed by the diagnostic laboratory system, wherein the first operation is one of a plurality of operations used to perform a first test on a sample; obtaining one or more second measurements during a second operation performed by the diagnostic laboratory system, wherein the second operation is one of the plurality of the operations used to perform the first test; collectively analyzing the one or more first measurements and the one or more second measurements using a trained model with learned correlations between the first operation and the second operation; determining an uncertainty score of the first test based on the collectively analyzing; and determining whether to rerun the first test based on the uncertainty score.
**2**. The method of claim 1, further comprising rerunning the first test in response to the uncertainty score being less than a predetermined value.
**3**. The method of claim 1, wherein: the obtaining one or more first measurements during the first operation comprises obtaining a first measurement having a value below an upper first measurement validity limit; the obtaining one or more second measurements during the second operation comprises obtaining a second measurement having a value above a lower second measurement validity limit; the collectively analyzing comprises collectively analyzing the first measurement and the second measurement using the trained model with learned correlations between the first operation and the second operation; and the determining an uncertainty score comprises determining a failing uncertainty score for the first test based on the collectively analyzing.
**4**. The method of claim 1, further comprising: encoding the one or more first measurements to a first vector representation that is representative of the first operation; and encoding the one or more second measurements to a second vector representation that is representative of the second operation.
**5**. The method of claim 4, wherein: the encoding the one or more first measurements comprises normalizing the one or more first measurements; and the encoding the one or more second measurements comprises normalizing the one or more second measurements.
**6**. The method of claim 4, wherein: the encoding the one or more first measurements comprises generating a reduced dimension vector from the one or more first measurements; and the encoding the one or more second measurements comprises generating a reduced dimension vector from the one or more second measurements.
**7**. The method of claim 1, wherein: the collectively analyzing the one or more first measurements and the one or more second measurements using the trained model with learned correlations between the first operation and the second operation comprises using a neural network to encode the one or more first measurements and the one or more second measurements into a vector space; and the determining the uncertainty score comprises determining the uncertainty score based on the vector space.
**8**. The method of claim 1, further comprising: representing a workflow of at least the first operation and the second operation as a graph having at least a first node and a second node, wherein the first node includes a vector representation of the one or more first measurements and the second node includes a vector representation of the one or more second measurements.
**9**. The method of claim 8, wherein: the collectively analyzing the one or more first measurements

and the one or more second measurements using the trained model with learned correlations between the first operation and the second operation comprises using a graph neural network to encode the graph into a vector space; and the determining the uncertainty score comprises determining the uncertainty score based on the vector space.

**10**. The method of claim 9, further comprising training the graph neural network on the workflow.

**11**. The method of claim 1, wherein the one or more first measurements comprise at least one of pressure, photometric, acoustic, temperature, and optical measurements.

**12**. The method of claim 1, wherein the first test is performed by a plurality of modules, and further comprising, in response to the uncertainty score being less than a predetermined value, determining which of the plurality of modules caused the uncertainty score to be less than the predetermined value.

**13**. The method of claim 1, further comprising, in response to the uncertainty score being less than a predetermined value, determining which of the first and second operations caused the uncertainty score to be less than the predetermined value.

**14**. A method of determining accuracy of tests performed by a diagnostic laboratory system, comprising: generating a graphical representation of a workflow of a test performable by the diagnostic laboratory system, wherein the graphical representation comprises a plurality of nodes and is configured to be analyzed by a graph neural network; obtaining one or more first measurements from a first operation performed by the diagnostic laboratory system during the test; converting the one or more first measurements to a first vector, wherein the first vector is a first node of the graphical representation; obtaining one or more second measurements from a second operation performed by the diagnostic laboratory system during the test; converting the one or more second measurements to a second vector, wherein the second vector is a second node of the graphical representation; analyzing the first node and the second node using the graph neural network; determining an uncertainty score of the test based on the analyzing; and determining whether to rerun the test based on the uncertainty score.

**15**. The method of claim 14, wherein: the diagnostic laboratory system is configured to perform a plurality of operations in a first sequence during the first operation; the diagnostic laboratory system is configured to perform a plurality of operations in a second sequence during the second operation; and the graph neural network is trained on the first sequence and the second sequence.

**16**. The method of claim 14, wherein: the converting the one or more first measurements comprises encoding the one or more first measurements to a first vector representation that is representative of the first operation; the converting the one or more second measurements comprises encoding the one or more second measurements to a second vector representation that is representative of the second operation, wherein the analyzing comprises collectively analyzing the first vector representation and the second vector representation using the graph neural network to map the first and second vector representations into a vector space; and determining the uncertainty score comprises determining the uncertainty score based on the vector space.

**17**. The method of claim 16, wherein the encoding comprises employing principal component analysis, independent component analysis or an auto encoder.

**18**. The method of claim 14, further comprising training the graph neural network on the workflow.

**19**. A diagnostic laboratory system, comprising: one or more modules configured to perform a test, the test having a workflow of a sequence of operations; a plurality of sensors configured to generate one or more measurements for each of the operations; a processor coupled to the sensors; and a memory coupled to the processor, wherein the memory includes a graph neural network and computer program code that, when executed by the processor, causes the processor to: generate a graphical representation of the workflow, wherein the graphical representation comprises at least a first node corresponding to a first operation of the workflow and a second node corresponding to a second operation of the workflow; convert one or more first measurements resulting from the first operation to a first vector, wherein the first vector corresponds to the first node; convert one or

more second measurements resulting from the second operation to a second vector, wherein the second vector corresponds to the second node; analyze the first vector and the second vector using the graph neural network; determine an uncertainty score of the test based on analyzing the first vector and the second vector; and determine whether to rerun the test based on the uncertainty score.

**20**. The diagnostic laboratory system of claim 19, wherein the memory includes computer program code that, when executed by the processor, causes the processor to: encode the one or more first measurements to the first vector that is representative of the first operation; encode the one or more second measurements to the second vector that is representative of the second operation; analyze the first vector and the second vector by using the graph neural network to map the first and second vectors into a vector space; and determine the uncertainty score based on the vector space.