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DEPARTMENT OF COMMERCE

National Institute of Standards and Technology

Existence and Use of Large Datasets to Address Research Questions for Characterization and Autonomous Tuning of Semiconductor Quantum Dot Devices

AGENCY: National Institute of Standards and Technology, U.S. Department of Commerce.

ACTION: Notice of workshop; request for comments.

SUMMARY: The National Institute of Standards and Technology (NIST) is seeking input regarding needs and gaps in data-sharing approaches to accelerate innovations in using artificial intelligence and machine learning techniques to improve the experimental characterization and control of semiconductor quantum dot devices. As part of this effort, NIST hopes to identify the needs for quantum dot device tuning automation, including existing and future quantum dot related datasets that may be useful for research, means and methods currently deployed for tuning, barriers for advancing the current state of the art techniques to enable automation of large quantum dot arrays, and the meaningful measures of success for the various stages of characterization and control. NIST plans to hold a workshop on July 19-20, 2023, in conjunction with this notice. The information received in response to this notice and during the workshop will inform efforts and coordination needed to develop a reference database of experimental and simulated data. The reference database will ideally represent the various phases of tuning quantum dot devices, along with metrics for benchmarking the characterization and control methods for quantum dot devices.

DATES:

For Comments: Comments must be received by 5:00 p.m. Eastern Time on [INSERT DATE 60 DAYS AFTER DATE OF PUBLICATION IN THE FEDERAL REGISTER]. Written comments in response to this notice should be submitted according to the instructions in the **ADDRESSES** section below. Submissions received after that date may not be considered.

For Workshop: The in-person Workshop on Advances in Automation of Quantum Dot Devices Characterization and Control will be held on July 19-20, 2023, from 9:00 a.m. to 5:00 p.m. Eastern Time at the National Cybersecurity Center of Excellence (NCCoE), 9700 Great Seneca Highway, Rockville, MD 20850. Attendees must register at the workshop website by 5:00 p.m. Eastern Time on June 19, 2023.

ADDRESSES:

For Comments: Written comments may be submitted only by email to Dr. Justyna Zwolak at aqd@nist.gov in any of the following formats: ASCII; Word; RTF; or PDF. Please include your name, organization's name (if any), and cite "Automation of Semiconductor Quantum Dot Devices" in the subject line of all correspondence. Comments containing references, studies, research, and other empirical data that are not widely published should include copies of the referenced materials. All comments responding to this document will be a matter of public record. Relevant comments will generally be made publicly available at *https://www.nist.gov/news-events/events/2023/07/advances-automation-quantum-dot-devices-control* as submitted. NIST will not accept comments accompanied by a request that part or all of the material be treated confidentially because of its business proprietary nature or for any other reason. Therefore, do not submit confidential business information or otherwise sensitive, protected, or personal information, such as account numbers, Social Security numbers, or names of other individuals.

For Workshop: The workshop will be held at NCCoE, 9700 Great Seneca Highway, Rockville, MD 20850. Please note admittance instructions under the **SUPPLEMENTARY INFORMATION** section of this notice. To register, go to: *https://www.nist.gov/news-events/events/2023/07/advances-automation-quantum-dot-devices-control.* Additional information about the workshop will be available at this web address as the workshop approaches.

FOR FURTHER INFORMATION CONTACT:

For questions about this notice contact Justyna Zwolak or Jacob Taylor by email at aqd@nist.gov or Justyna Zwolak by phone at (301) 975-0527. Please direct media inquiries to NIST's Office of Public Affairs at (301) 975-2762.

SUPPLEMENTARY INFORMATION:

Background: Over the past five years, researchers working with semiconducting quantum dot devices have begun to take advantage of the data analysis tools provided by the field of artificial intelligence and, more specifically, supervised and unsupervised machine learning. When provided with proper training data, machine-learning-enhanced methods may have the flexibility of being applicable to various devices without any adjustments or retraining. Moreover, by learning the governing rules and dynamics directly from the data, machine learning algorithms may be less susceptible to programming errors. However, machine learning models typically require large, labeled datasets for training, validation, and benchmarking. They also often lack information about the reliability of the machine learning prediction. Moreover, since the application of machine learning to quantum dot tuning, characterization, and control is a relatively new field of research, it lacks standardized measures of success. The success rates reported in the various publications vary significantly in both the level and meaning of the reported performance statistics, making it hard (if not impossible) to benchmark the proposed techniques against more traditional tuning approaches or against one another.

Through this notice, we seek public comment to identify existing large datasets that may be useful for research; identify best practices for creating new, large datasets that are valuable for research; understand the challenges and limitations that may impact data access; and current and future key metrics of performance for the tuning methods.

Request for Comments

The following statements are not intended to limit the topics that may be addressed. Responses may include any topic believed to have implications for the development of auto-tuning methods for semiconductor quantum dot devices, regardless of whether the topic is included in this

document. All relevant responses that comply with the requirements listed in the **DATES** and **ADDRESSES** sections of this notice will be considered.

NIST seeks input from stakeholders regarding the broadly defined needs for automation of quantum dot device characterization and tuning. A simple but crucial component of success for the field will be to solidify key metrics of performance as well as establish standard datasets that can be used to assess those metrics on the newly proposed methods and algorithms. Among the simple metrics that have been used to date are state identification accuracy (probability of a classifier identifying the right topology) and tuning success (probability of the navigation algorithm getting to the right region of parameter space). However, more such metrics, and associated datasets, will be necessary to leverage machine learning algorithms most effectively. So far, machine learning efforts for semiconductor quantum dots rely on datasets that either come from simulations (and thus may lack important features representing real-world noise and imperfections) or are labeled manually (and subject to qualitative and/or erroneous classification). Moreover, with a few exceptions, these datasets are not made publicly available. Yet, systematic benchmarking of tuning methods on standardized datasets, analogous to the MNIST or CIFAR datasets in the broad machine learning community, is a crucial next step on the path to developing reliable and scalable auto-tuners for quantum dot devices.

Through this notice, we seek public comment to initiate a community-wide effort to build an open-access data repository for benchmarking automated methods for quantum dot devices. To initiate such efforts, NIST has provided a starting point: an open dataset, *QFlow*, hosted at the NIST science data portal www.data.nist.gov, that includes a large number of simulated measurements as well as a small set of experimental scans. A standardized dataset that would enable systematic benchmarking of the already existing and new auto-tuning methods should represent data from different types of devices. This standardization work will take time and community engagement, based on experience from other machine learning disciplines. Once standardization is in place, more algorithmic exploration and improvement can be achieved.

We invite any member of the public, and specifically those who are aware of datasets relevant to auto-tuning quantum dot devices or interested in establishing a large open-access database of experimental data; those who have perspectives on the value of these datasets for research; and those who are aware of challenges and limitations to both access and use of large datasets to share their input on the following points in their comments:

(1) Identify public or restricted use datasets related to the various phases of tuning semiconductor quantum dot devices that are available for training and benchmarking new artificial intelligence models or to test hypotheses using data mining/machine learning methods. Describe the research needs that are not being met by the datasets that are currently available.

(2) Describe the work researchers need to do to access, and then explore the quality of, an existing dataset before conducting research with it. Identify what aspects of this work could be reduced or conducted just once so that future researchers can reduce the time needed to complete a research project.

(3) Describe promising approaches to testing and improving the validity of performance metrics within large datasets, especially those datasets that consist of experimental data that does not come with ground truth labels.

(4) Describe whether existing datasets, both simulated and acquired experimentally, contain data that are valuable for researchers and are of sufficient quality that research could be conducted with a high amount of rigor.

(5) Describe to what extent existing datasets capture enough information to address research related to all aspects of tuning quantum dot devices. Identify what additional data should be collected to address these research questions.

(6) Describe the best practices for creating new datasets or linking existing datasets and sharing them with researchers (open or restricted use) while adhering to local, State, and Federal laws. Identify barriers and limitations that currently exist.

(7) Describe what role NIST can play in developing infrastructure that supports the use of large-scale datasets for research on tuning quantum dot devices

Workshop

The purpose of the workshop is to convene stakeholders from industry, academia, and the government interested in the research and development of semiconductor quantum computing technologies. Topics to be discussed include opportunities for research and development of tuning, characterization, and control methods for semiconductor quantum dot devices, the need for facilitating interaction and collaboration between the stakeholders to build a large open-access database of experimental and simulated data for benchmarking new machine learning algorithms, determining key performance metrics for the various aspects of the tuning, characterizing, and controlling of quantum dot devices, and identifying barriers to near-term and future applications of the auto-tuning methods. Furthermore, this workshop will provide a discussion place to consider methods of collaboration in a neutral setting and future roadmap development for methods for tuning large-scale devices.

This workshop will focus on addressing the key challenges described above under "Request for Comments." It will include invited presentations by leading experts from academia, industry, and government; time for group discussion; and breakout sessions for discussing questions (1) through (7). No proprietary information will be accepted, presented or discussed as part of the workshop, and all information accepted, presented or discussed at the workshop will be in the public domain.

More information about the workshop can be found at *https://www.nist.gov/news-events/events/2023/07/advances-automation-quantum-dot-devices-control*. All participants must pre-register to be admitted. Also, please note that federal agencies, including NIST, can only accept a state-issued driver's license or identification card for access to federal facilities if such license or identification card is issued by a state that is compliant with the REAL ID Act of 2005 (Pub. L. 109-13), or by a state that has an extension for REAL ID compliance. NIST currently

accepts other forms of federally-issued identification in lieu of a state-issued driver's license. For detailed information please contact Meliza Lane at elsie.lane@nist.gov or by phone (303) 497-5356 or visit: *http://www.nist.gov/public_affairs/visitor/.*

Authority: 15 U.S.C. 272(b) & (c); 15 U.S.C. 278h–1.

Alicia Chambers,
NIST Executive Secretariat.
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