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Phys. Rev. Applied **19**, 054077 — Published 24 May 2023

DOI: 10.1103/PhysRevApplied.19.054077

Automated extraction of capacitive coupling for quantum dot systems

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Gate-defined quantum dots (QDs) have appealing attributes as a quantum computing platform. However, near-term devices possess a range of possible imperfections that need to be accounted for during the tuning and operation of QD devices. One such problem is the capacitive cross-talk between the metallic gates that define and control QD qubits. A way to compensate for the capacitive cross-talk and enable targeted control of specific QDs independent of coupling is by the use of virtual gates. Here, we demonstrate a reliable automated capacitive coupling identification method that combines machine learning with traditional fitting to take advantage of the desirable properties of each. We also show how the cross-capacitance measurement may be used for the identification of spurious QDs sometimes formed during tuning experimental devices. Our systems can autonomously flag devices with spurious dots near the operating regime which is crucial information for reliable tuning to a regime suitable for qubit operations.

I. INTRODUCTION

Quantum dot (QD) arrays, in which charge carriers 34 are trapped in localized potential wells and qubits can 35 be made by use of the spin and permutation symmetries 36 of the carriers, are a promising quantum computing plat- 37 form [1–3]. In fact, last year has shown the first demon-38 stration of QD two-qubit gates with fidelities exceeding 39 the thresholds for fault-tolerant computing [4–6]. How- 40 ever, because the individual charge carriers that makeup 41 qubits have electrochemical sensitivity to minor impu-42 rities and imperfections, calibration and tuning of QD 43 devices is a nontrivial and time-consuming process, with 44 each QD requiring a careful adjustment of a gate voltage 45 to define charge number, and multiple gate voltages to 46 specify tunnel coupling between QDs for two-qubit gates 47 or to reservoirs for reset and measurement. While manual $^{48}\,$ calibration is achievable for small, few-QD devices, with 49 increasing size and complexity of QD arrays, the relevant 50 control parameter space grows quickly, necessitating the 51 development of autonomous tuning methods.

There have been numerous demonstrations of automa- ⁵³ tion of the various phases of the tuning process for sin- ⁵⁴ gle and double-QD devices [7]. Some approaches seek to ⁵⁵ tackle tuning starting from device turn-on to coarse tun- ⁵⁶ ing [8–11] while others assume that bootstrapping (cal- ⁵⁷ ibration of measurement devices and identification of a ⁵⁸ nominal regime for further investigation) and basic tun- ⁵⁹ ing (confirmation of controllability and device character- ⁶⁰ istics) have been completed and focus on a more tar- ⁶¹ geted automation of the coarse and charge tuning [12–16]. ⁶² While the initial auto-tuning approaches relied mainly ⁶³

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on the appealingly intuitive and relatively easy to implement conventional algorithms that typically involved a combination of techniques from regression analysis, pattern matching, and quantum control theory, the more recent algorithms take advantage of the modern computer vision and machine learning [7].

A typical accumulation-mode QD device consists of two sets of gates—plungers and barriers—that collectively control the overall potential profile, QD-specific single-particle energy detuning of individual QDs, the tunnel couplings between QDs, and tunnel rates between the most outer QDs and reservoirs. Ideally, each plunger gate would affect only the electrochemical potential of a single targeted QD and each barrier gate only one intended tunnel barrier. Due to the tight proximity, however, each gate capacitively couples to nearby potential and tunnel barriers. This makes careful control of these key parameters challenging.

One way to compensate for the capacitive cross-talk between gates is to enable orthogonal control of the QDs potential by implementing so-called *virtual gates* [17]. Specifically, linear combinations of gate voltage changes can be mapped onto onsite energy differences [17–20]. These approaches have been key for the initialization and control of larger QD arrays [21, 22].

To autonomously identify capacitive couplings in a device, various approaches have been demonstrated using both conventional fitting and machine learning (ML) techniques [23–26]. However, these approaches, typically relying on the Hough transform or conventional least-squares fitting procedures, may be unreliable in the presence of data imperfections. Hough transforms can extract slopes directly but may be sensitive to noise or be excessively complex to analyze. The conventional fitting can be more flexible but is susceptible to local minima and can be time-consuming at inference time.

Convolutional neural networks (CNN) are well suited for extracting high-level features from images and can

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remain effective in the presence of noise or other imperfections [27]. However, ML methods can have difficulties identifying data outside of the training distribution even if it contains similar features [28]. Fortunately, given a simplified, high-level representation of the data, conventional fitting approaches can be more targeted to extract key information more effectively and quickly.

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Here we develop a reliable automated capacitive coupling identification method that combines ML with traditional fitting to take advantage of the desirable properties of each. We use an ML module for pixel classification followed by linear regression for extracting targeted information and demonstrate effective performance across noise levels and data variations. Testing each of these methods on a set of eight simulated QD devices with large variability and realistic noise variation mimicking experimental conditions shows that the approach combining ML and traditional fitting works well, with a root mean square error (RMSE) of 0.034(14), corresponding to a roughly 8 % error, for predicting virtual gate matrix off-diagonal values (normalizing such that diagonal values are one) [29]. This RMSE roughly corresponds to the error rate expected for previous cross-capacitance extraction methods [24] that required multiple iterations and higher data quality.

We also demonstrate how the cross-capacitance measurement may be used for the identification of spurious QDs formed during tuning experimental devices. Many $_{56}$ of the auto-tuning approaches proposed to date rely on 57 a series of small 2D scans capturing a relatively narrow 58 range of the voltage space [13, 14, 27, 30]. While such ap-50 proaches improve the efficiency of tuning, they may result $_{60}$ in unexpected and difficult to assess failure modes when 61 the tuning algorithm terminates at an anti-crossing with 62 a spurious QD that may form in small potential wells due $_{63}$ to interface defects, surface roughness, or strain within 64 the device [31]. They are highly undesirable since they 65 may interfere with the QDs intended for use as qubits $_{66}$ and cannot themselves be used as qubits. To avoid de-67 vice tuning failure, spurious QDs must be identified when $_{68}$ present and avoided. We test the utility of our approach $_{69}$ for capacitive coupling estimation by identifying spurious 70 QD in experimental measurements of QD devices [1].

The manuscript is organized as follows: In Sec. II we $_{72}$ introduce the framework of combining traditional fitting $_{73}$ techniques with a pixel classifier to process the high-level $_{74}$ information extracted from experimental data. In Sec. III $_{75}$ we show the utility of the proposed framework to auto- $_{76}$ matically extract virtual gates as well as identify charge $_{77}$ transitions resulting from a formation of spurious QD. $_{78}$ Finally, in Sec. IV we summarize the results and discuss the outlook.

II. METHODS: MACHINE LEARNING AND FIT

Capacitive couplings in a QD device can be measured 81 and, in a constant capacitance approximation, described 82

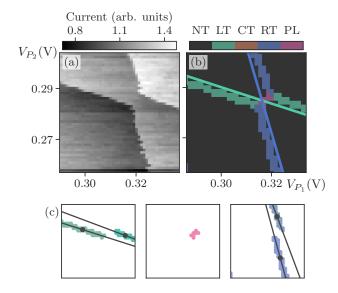


FIG. 1. An example 2D scan and corresponding pixel classification, class clusters, and linear fits. (a) A simulated voltage scan showing left and right transitions as well as a polarization line. (b) Pixel classification for the scan shown in (a). (c) Regions of pixels and linear fits from the pixel classification. The large dark points indicate the centers of pixel regions.

by a matrix that maps the physical gate voltages onto the effect they each have on the QD's chemical potentials or barriers [17, 23, 24, 32–34]. Measurement of the elements of this matrix must be performed distinctly for electrochemical potentials and tunnel barriers. Couplings of the chemical potentials to each QD—which is the focus of this work—can be extracted from shifts in charge transition lines when each voltage is varied [17] while the effect of each gate on tunnel barriers can be assessed by measuring changes in the width of inter-dot transitions, assuming the electron temperature is sufficiently low [33]. Measured this way, the couplings are relative, usually scaled with respect to the coupling of the QD to the nearest gate. An absolute energy scale can be obtained by measuring the gate lever arms with photon-assisted tunneling, Coulomb diamonds, or bias triangles [35]. However, for establishing the orthogonal control the relative scale is sufficient [21].

For a double QD, the virtualization matrix relating the physical plunger gates to virtual gates can be represented by Eq. 1. Each row is normalized such that the diagonal entries are 1 to reflect the relative nature of our virtual gates.

$$\begin{pmatrix} V_{P_1'} \\ V_{P_2'} \end{pmatrix} = \begin{pmatrix} 1 & \alpha_{12} \\ \alpha_{21} & 1 \end{pmatrix} \begin{pmatrix} V_{P_1} \\ V_{P_2} \end{pmatrix} \tag{1}$$

The relative cross-capacitances for chemical potentials manifest themselves via the slopes of charge transition lines, with the dominant terms of the cross-capacitance matrix determined from a measurement in the space of neighboring pairs of gates [21]. We address the identification of the cross-capacitances as captured in twodimensional (2D) plunger-plunger gate scans, as shown in Fig. 1(a). To translate the low-level QD data into high-level information useful for automation we use a pixel classifier, i.e., a CNN model with a structure similar to a feature pyramid network [36]. Additional details about the CNN design can be found in Appendix A. The pixel classifier takes as an input a small 2D plunger voltage scan obtained using a charge sensor, as shown in Fig. 1(a). It then identifies each pixel within the scan as belonging to one of the charge transition classes—that of left QD, right QD, central QD, or inter-dot (polarization line) transition, denoted as LT, RT, CT, or PL, respectively—or to the no transition (NT) class. In other words, the CNN provides a high-level classification of the raw experimental data while keeping spatial information about the relative location and orientation of the detected features, which is useful for algorithmic processing. Figure 1(b) shows the pixel classification of a scan from Fig. 1(a).

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To translate pixel classifications to capacitive couplings, we identify contiguous regions within each class of pixels in an image and then independently fit them using a linear regression model. A labeling algorithm from the multidimensional image processing package in SciPy is then used to determine the relevant clusters of connected pixels for each class [37]. This separates charge transitions into distinct lines identified by an index and an assigned class so that each can be processed individually. The x and y pixel indices of each region of pixels $_{_{\rm EE}}$ classified as LT, CT, or RT are independently fitted using $\tilde{}_{56}$ linear regression, as shown in Fig. 1(c). When multiple segments for a given class are present in an image, the capacitive coupling returned is the average for all fitted lines weighted by the number of pixels in each cluster and the standard deviations of the respective fits, yielding the solid lines in Fig. 1(b) (offset arbitrarily for comparison with the pixel regions). To facilitate a more direct calculation of the fit error for the RT capacitive coupling, the x and y indices are inverted before linear regression. Standard deviations σ are computed from the standard error of the fit, S, by $\sigma = S/\sqrt{n}$, where n is the number of pixels in the pixel region, as in Student's t-distribution [38]. In addition, each region is tagged with its center in voltage space, shown by the large black points in Fig. 1(c), which allows tracking the changes in charge transitions and their slopes within the larger space.

A. Data

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The data used for training the ML tools and testing 77 the methods was generated using a simulation of QD de- 78 vices [12]. The simulation is composed of a calculation of 79 the electron density in the Thomas-Fermi approximation 80 and a capacitance matrix to determine the stable electron 81 configuration. To improve the robustness of the models, 82

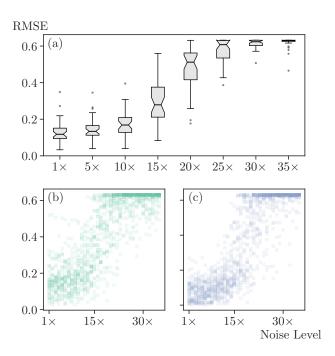


FIG. 2. (a) Box plot of root mean square error (RMSE) for all transition classes (left, central, and right [LT, CT, RT]) as a function of the synthetic noise level. The notch indicates the 95 % confidence level. (b) RMSE as a function of noise level for the LT class. (c) RMSE as a function of noise level for the RT class.

the data is augmented with synthetic white, pink (1/f), and telegraph noise [27]. The effect of a QD charge sensor strongly coupled to the plunger gates is varied during the scan to improve performance on this type of experimental data.

The training dataset consists of 1.6×10^5 devices with parameters varied over a uniform distribution with a standard deviation equal to 1 % of each parameter's value. To train the ML models we randomly sample 10 small scans per device and use charge state ground truth to label each scan on a pixel level with the presence and type of transition, yielding NT, LT, CT, RT, and PL labels. Additionally, we extract the slopes of the transition lines directly using the gradients of the device charge.

The test data consists of eight simulated devices with large variations in screening length and device pitch and with large shifts in the position of one of the plunger gates. These changes lead to large variations in the slopes of and spacing between the charge transition lines, the capacitive coupling between QDs, and the relative sizes of left and right QD regions, making them largely distinct from the training data. To facilitate a controlled study and track the performance of the pixel classifier as data quality degrades, each large scan is randomly sampled 50 times and the resulting small scans are augmented with increasing levels of synthetic noise. This results in a set of 400 simulated test scans. Finally, several large experimental measurements acquired using a double-QD

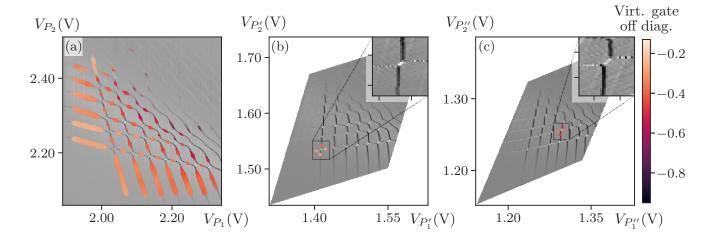


FIG. 3. (a) Large experimentally measured charge stability diagram with a scatter plot of centers of pixel class regions overlaid. The colors of the points indicate the virtual gate off-diagonal values identified by fits to the region. The sizes of the points indicate the weights used when averaging. Only points with relative error less than 20 % are plotted. (a,b) Charge stability diagram after applying virtual gates acquired near the (0,0)-(1,1) charge transition in (a) and near the (1,3)-(2,4) charge transition in (b). In both (b) and (c) the virtualization is performed off-line, via an affine transform to the original scan shown in (a) and the points are plotted using the same parameters as in (a).

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configuration on a three-QD $\mathrm{Si}_x/\mathrm{SiGe}_{1-x}$ device, fabri- 30 cated on an industrial 300 mm process line [1], are used 31 to test the performance of the virtualization algorithm. 32 Experimental scans capturing spurious QDs are used to 33 demonstrate the algorithm for spurious QD detection. 34

III. RESULTS

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We test the effectiveness of our automated approach to 40 extracting the cross-capacitance by first evaluating the 41 performance of each component, i.e., the pixel classifier 42 and the slope extractions, on each scan in the simulated 43 test set. The error of the pixel classifier in our framework 44 is defined as a fraction of pixels belonging to true transi- 45 tions that are not contained in line segments in the CNN output. This captures type II errors (false negatives) without the effect of false type I errors (false positives) due to imperfect labels [39]. Figure 2(a) shows the change 46 in RMSE of the extracted off-diagonal virtual gate values as a function of the noise level in the simulated data. At 47 the noise level of 1.0, i.e., the noise level estimated from 48 experimental data in Ref. [30], we observe an RMSE of 49 0.17(5). The RMSE increases significantly to 0.50(11) 50 at the noise level of 20. For reference, a pixel classifier 51 that always predicts the NT class would have an RMSE 52 of 0.62 ($\sqrt{0.4}$). For the LT and RT classes relevant to 53 cross-capacitances, shown in Fig. 2(b) and (c), the pixel 54 classifier for noise level 1.0 has an RMSE of 0.20(8) and $_{55}$ 0.11(8), respectively.

To verify that the slope extraction tool works as in- $_{57}$ tended, we test it across the eight large simulated test $_{58}$ devices. For these tests, we evaluate the pixel classifier $_{59}$

in windows of size roughly $1.5\times$ the charging energy, as estimated by the spacing of the first two charge transitions. Outputs from the pixel classifier are cropped by one pixel from the edge of the image before processing because the zero-padding at each layer causes reduced performance at image edges [40]. The resulting classes of pixels are then grouped into distinct clusters. For each cluster consisting of more than five pixels an independent linear fit is performed, returning both the slope and the standard error of the fitted line. The RMSE for the linear fits compared to the cluster from pixel classifications is 0.6 pixels, which is near the minimum relative to the two-pixel width of lines in pixel classifications. This information can be used to find the orthogonal "virtual" control space or to flag transitions that potentially belong to spurious dots, as described in the following sections.

A. Deriving virtual gates

As stated in Sec. II, we derive the off-diagonal elements of the capacitance matrix (defining the virtual gates transformation) based on the slopes of the LT and RT captured in a given image, while the diagonal elements are set 1.0. When multiple lines belonging to the same class are detected, as in Fig. 1(a), the capacitive coupling is calculated through a weighted average [38].

The off-diagonal elements of the virtualization matrix computed this way have an RMSE of 0.034(14) at the noise level of 1.0 defined in Ref. [30], corresponding to a roughly 8 % error compared to the ground truth values derived from simulated data. We further test them on a range of levels of synthetic noise and find the RMSE

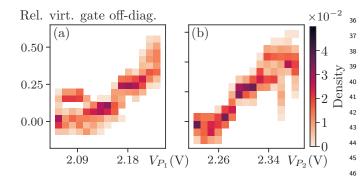


FIG. 4. Histograms of the off-diagonal elements of the virtualization matrix for an experimentally measured scan shown sin Fig. 3(a) as a function of plunger gates, (a) V_{P_1} and (b) so V_{P_2} . Off-diagonal values are shifted and scaled by the mean so of the off-diagonal elements from virtual gates in the (1,1) sharper state for ease of comparison. Virtual gate values are sextracted from a strip of small scans shifted by 3 mV (two sapixels) in each opposing direction to better visualize variation state ach plunger gate value.

rises by a factor of two at a level of noise of roughly $15 \times$ 58 the level of noise defined in Ref. [30], consistent with the 59 pixel classifier error.

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To better understand the trends of the virtualization matrix in the plunger-plunger space, we carry out a performance analysis using the simulated test set and several experimentally measured scans. For each scan, we calculate the fits to the pixel classification clusters based on a series of small scans sampled at each point within the large scan with the exclusion of a margin implemented 65 to ensure that all sampled scans fall within the full scan boundaries. The small scans and the margins are set to 66 have a size $1.5\times$ the charging energy of a given simu- 67 lated device. Figure 3(a) shows the centers of the pixel 68 region identified in each small scan [as in Fig. 1(c)] as the 69 sampling window is swept across a large experimentally 70 measured charge stability diagram. The regions iden-71 tified by the pixel classification are consistently placed 72 correctly on the charge transition lines regardless of the 73 position of the line within a small scan. Region centers 74 shift along the charge transition lines as different por-75 tions of the line are captured within the small scan and 76 remain fixed whenever the same fragment of the charge 77 transition is captured. The color of the points indicates 78 the off-diagonal values of the virtual gate matrix, α_{12} and 79 α_{21} . As expected, these coupling constants get larger in ∞ magnitude as charges are added to each QD. Finally, the 81 size of the points in Fig. 3(a) indicates the $1/\sigma^2$ weight of 82 the slopes used when averaging multiple slopes from the 83 same type of transition within a small scan. As desired, 84 the positions of the points with smaller sizes indicate that 85 lines that are smaller or less captured within a small scan 86 have fits with larger errors. Overall, this plot confirms 87 that the combination of pixel classification with the fits is 88 working as intended at capturing charge transition lines 89 and their slopes.

To demonstrate the spatial relevance of the virtual gates derived from a set of fits across a device's charge landscape, in Fig. 3(b) and (c) we plot affine-transformed charge stability diagrams, with points indicating fits overlaid. The points plotted are the centers of pixel regions with the same color and size encoding as in (a). The affine transformation applied in Fig. 3(b) corresponds to virtual gates derived from an image near the (0,0)-(1,1) charge transition with off-diagonal values $\alpha_{12} = -0.282(4), \ \alpha_{21} = -0.331(4).$ For Fig. 3(c), the affine transformation applied has virtual gates from the (1,3)-(2,4) charge transition, with off-diagonal values $\alpha_{12} = -0.363(4), \ \alpha_{21} = -0.480(4).$ As can be seen in the insets in Fig. 3(b) and (c), these virtual gates are very effective at transforming the target region to an orthogonal space, but the difference between the extracted virtual gate off-diagonal values are about 50 % higher for the latter case. This highlights the importance of an efficient local method for determining virtual gates.

To further understand how capacitive coupling varies across a charge stability diagram, we can calculate variation as each plunger gate is adjusted. Figure 4(a) and (b) show how cross-capacitances extracted from small scans change as V_{P_1} and V_{P_2} are varied. To better show the trend of expected values, cross-capacitances from small scans shifted by 3 mV (two pixels) in each opposing direction are included. This shows that the cross-capacitances extracted from small scans effectively capture variation across charge stability diagrams.

B. Detection of spurious dots

Visually, spurious QDs are recognized in large 2D scans as charge transitions with slopes diverging from a monotonic trend. In this framework, they may be identified as transition lines with anomalous capacitive couplings relative to the transitions around them.

As a demonstration, we use the pixel classification and fit tools to analyze five experimental charge stability diagrams: two capturing properly formed QD, shown in Fig. 5(a) and (b), and three capturing spurious QDs, shown in Fig. 5(c), (d), and (e). While for extraction of the virtualization matrix small scans are sufficient, detection of spurious QD requires somewhat bigger scans to ensure that the neighboring charge transitions are adequately captured. In our analysis, we rely on 2D scans of a size roughly three times the charging energy (four times the area of scans typically used in auto-tuning algorithms [13, 14]). We also consider only clusters consisting of at least 20 pixels to ensure better reliability of the linear fit.

After pixel classification, contiguous clusters of pixels belonging to a given class of transitions are analyzed individually, resulting in a cluster-based fit and standard deviation. Cases where more than one cluster belongs to a given charge transition result in separate fits, as in Fig. 5(b) and (e) where the LT lines are split into groups

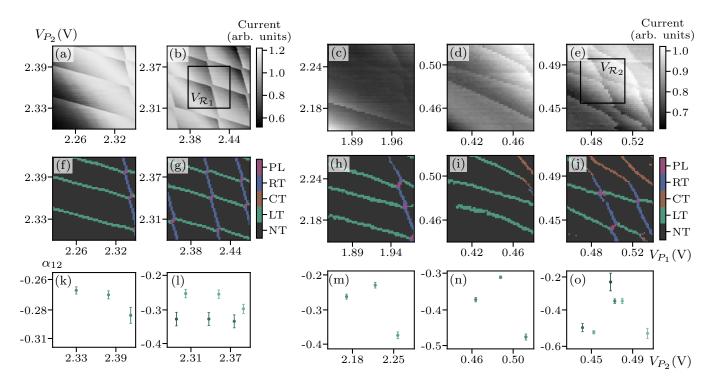


FIG. 5. Spurious dot detection. The top row shows two charge stability diagrams capturing properly formed QD [panels (a) and (b)] and three charge stability capturing spurious QD [panels (c), (d), and (e)]. The black boxes in (b) and (e) highlight small 2D scans, denoted as $V_{\mathcal{R}_1}$ and $V_{\mathcal{R}_2}$, typical of the auto-tuning approaches proposed in Ref. [13, 14]. Panels (f)–(j) in the middle row show pixel classification results for charge stability diagrams shown in the top row. Plots of fitting results used to determine whether a spurious QD is present are shown in the bottom row [panels (k)–(o)]. The different groups of transition are shown with different shades of green. The monotonicity within each group of transitions is clearly visible in panels (k) and (l). On the contrary, in the three plots shown in panels (m), (n), and (o), there is a clear divergence from the expected trend for the spurious QD, as indicated by the non-monotonic change between the first (most left point) and second (middle point) transition. Error bars indicate one standard deviation.

to either side of the RT lines. This separation serves two ²⁴ purposes: to ensure that variation along a given transi- ²⁵ tion isn't included and to treat each additional line inde- ²⁶ pendent of the charge on another QD.

Within a class and group of transitions, the magnitude ²⁸ of the capacitive coupling is expected to increase mono- ²⁹ tonically while the spacing between consecutive transi- ³⁰ tion lines decreases as a charge is added. Such behavior is ³¹ clearly visible in Fig. 5(k) and (l), with the latter having ³² to separate groups of fits (shown with different shades of ³³ green) for the groups of clusters. On the contrary, a spu- ³⁴ rious QD can manifest itself by a non-monotonic behav- ³⁵ ior of the capacitive coupling between transitions. This ³⁶ is depicted graphically by either the most left or the cen- ³⁷ ter point (or group of points) not following the expected ³⁸ decreasing trend in Fig. 5(m), (n), and (o). The severity ³⁹ of this divergence can be quantified using a Z-test [41].

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In practical applications, the automated detection of spurious QD fits nicely within the auto-tuning paradigm. As mentioned earlier, many of the proposed approaches tutilize a series of small 2D scans [13, 14, 27, 30] or 1D rays [42, 43] as means to improve the tuning efficiency. While these approaches deliver measurement-scot-effective solutions, they are prone to unexpected and 15 spurious quantum detection of the spurious three detections.

difficult-to-detect failure even when the data quality is high. Fig. 5(b) and (e) show examples of such potentially problematic cases. The small 2D regions in the plungerplunger space, highlighted in these scans with the black boxes, are typical for topology setting algorithms. In both cases, they are classified by a state classifier model as double QD state, with state prediction vectors being $p(V_{\mathcal{R}_1}) = [0.01, 0.04, 0., 0.04, 0.92]$ for $V_{\mathcal{R}_1}$ region highlighted in Fig. 5(b) and $p(V_{\mathcal{R}_2}) = [0., 0., 0.18, .05, 0.76]$ for region $V_{\mathcal{R}_2}$ highlighted in Fig. 5(b), where $p(V_{\mathcal{R}}) =$ $[p_{\mathrm{ND}},\,p_{\mathrm{SD}_L},\,p_{\mathrm{SD}_C},\,p_{\mathrm{SD}_R},\,p_{\mathrm{DD}}]$ with ND denoting no QDs formed, SD_L , SD_C , and SD_R denoting the left, central, and right single QD, respectively, and DD denoting the double-QD state. Moreover, the data quality for these images is high in both cases, with $q(V_{\mathcal{R}_1}) = [1.0, 0.0, 0.0]$ for region $V_{\mathcal{R}_1}$ and $q(V_{\mathcal{R}_1}) = [0.99, 0.01, 0.0]$ for $V_{\mathcal{R}_2}$, where $q(V_R) = [p_{high}, p_{mod}, p_{low}]$ with p_{high}, p_{mod} , and p_{low} denoting the probability of region $V_{\mathcal{R}}$ being assessed by the data quality control module as "high,", "moderate," and "low" quality, respectively. Thus, from the ML perspective, both these predictions are confidently correct. However, when looked at within a slightly larger voltage range, it is clear that in the latter case, the small scan captures an anti-crossing with a spurious QD.

which for practical tuning purposes is a failure. If not ³⁸ recognized and corrected for, termination at this point will result in an incorrect charge setting and virtualization [13, 30].

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The spurious QD detection algorithm can be easily implemented in the auto-tuning algorithm proposed in Ref. [27] as a safety check before the unloading step is initiated. If a transition is flagged as potentially problematic, tuning may be suspended and measurements on other gates initiated to further investigate the problem. Additional analysis to determine the separation between transitions can be implemented as a measure complementary to the monotonicity analysis. Automated identification and characterization of spurious QDs may also be useful to inform fabrication procedures and prevent them in future devices [31].

IV. CONCLUSIONS

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As QD devices grow in size and complexity, the need 55 for reliable and automated tune-up procedures becomes 56 more pressing. Establishing orthogonal control of the 57 chemical potentials of QDs is one of the first steps in 58 the tune-up of any larger QD array. Here, we demon- 59 strated a method that combines machine-learning-based $_{60}$ pixel classification and traditional curve fitting to reli- 61 ably determine voltage cross-talk coefficients. The ad- 62 vantage of this method over previous approaches is high- 63 lighted by increased reliability and resilience to experi- 64 mental noise. Further on, unwanted spurious dots that 65 would reduce or inhibit device performance can be de-66 tected and flagged when this module is used as part of a 67 larger tune-up algorithm [30]. The capability to automat- 68 ically and reliably detect spurious dots is especially im- 69 portant on wafer-scale fabrication characterization tools 70 that produce more data than can efficiently be processed 71 by human analysis. In extensions, our tools could allow 72 for automated navigation of voltage space for more tar-73 geted measurement of all chemical potential and tunnel 74 barrier cross-capacitances [17, 33].

ACKNOWLEDGMENTS

This research was performed while J.Z. held a NRC Research Associateship award at the National Institute of Standards and Technology (NIST). The views and conclusions contained in this paper are those of the authors and should not be interpreted as representing the official policies, either expressed or implied, of the U.S. Government. The U.S. Government is authorized to reproduce and distribute reprints for Government purposes notwithstanding any copyright noted herein. Any mention of commercial products is for information only; it does not imply recommendation or endorsement by NIST.

Appendix A: The structure of the CNN

The CNN used in the pixel classifier model follows an architecture similar to a feature pyramid network [36] with separable convolutions in the downsampling branch, residual connections, and batch normalization applied after each convolution and activation. This structure is adapted from an example in Ref. [44], with the major difference being long skip connections between the upsampling and downsampling branches of the network. The downsampling branch has three pairs of convolutional layers of kernel size three and 16, 32, and 64 filters with residual connections between the input and output of each pair. Residuals are computed using a 1×1 convolution followed by addition. Each pair of convolutions is followed by a max pooling layer with a stride two. The upsampling branch similarly has three pairs of transpose convolutional layers with 64, 32, and 16 filters, with residual connections between the input and output of each pair. Each pair of convolutions is followed by an upsampling layer with stride two. Long skip connections go between the output of each downsampling layer to the output of each upsampling layer with a matching number of the image size using a convolutional layer of kernel size three. The CNNs are trained using the Adam optimizer [45] with a learning rate 1×10^{-3} .

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