k-nearest neighbors algorithm-assisted transport measurement

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I. PURPOSE OF KNN ALGORITHM

The k-nearest neighbors algorithm (KNN) can be used to characterise a quantum-dot based single-electron pumps[1]. The concept of a single-electron pump[2] follows the definition of the SI unit of current, the ampere (A)[3]. One of the advantages of single-electron pumps is their relative accuracy at the level of current magnitude of 10^{-7} A. The world record of the relative accuracy for this device is $\sim 2 \times 10^{-7}$[4]. Without the help of KNN, electron transport measurements for the accuracy assessment of single electron pumps are time consuming depending on the accuracy level. It has been shown that KNN algorithm can reduce the time taken to assess the pumping accuracy by multiple times[1].

Typically, the scanning parameters consist of two gate voltages, such as V_1 and V_2. By scanning the parameter space of V_1 and V_2, a two-dimensional current density plot can be generated. The relative accuracy of the single-electron pump is evaluated by analyzing the slope of the current plateau region in the density plot which is call pumping map. The program with the KNN algorithm performs measurements of the current, I vs V_1 and V_2. ~~In addition, the measurements of dI/dV_i vs V_1 and V_2 are also performed, where $i = 1, 2$.~~

II. EXPERIMENTS AND RESULTS

We present a preliminary dataset to show the feasibility of our program. Using a quantum point contact (QPC) device which can be realized by making active a pair of gates of a quantum dot whose geometry is similar to our previous one[2], we show that the KNN algorithm is suitable for our purposes. The QPC features conductance quantization as $n \times G_0$ where $G_0 = 2e^2/h$ and n is an integer while the pump device features quantized current steps as $I = nef$ where f is the pumping modulation frequency[2]. Figure 1 describes 3D plots of current I vs V_{g1} and V_{g2} as well as current heatmap investigated at $T = 4.2$ K. They manifest current steps due to the conductance quantization. The minus sign of the current is attributed to the reversed polarity of the current amplifier.

Although not shown here, the KNN dI/dV_i algorithm is also an efficient tool for identifying current/conductance plateaus during the scanning of gates V_1 and V_2, while also reducing measurement time. Compared to KNN I vs V_i measurement, its derivative along the parameter space could provide a better contrast in the current heatmap.

Figure 2(a) compares currents measured I^{m} and obtained I^{KNN} by KNN algorithm with their standard deviations σ^{m} and σ^{KNN}, respectively. Both σ's show oscillating curves making peaks and valleys matching the current slope and plateau regions, respectively. We believe that the main origin of the uncertainty (σ^{m} and σ^{KNN}) is attributed to the instability of the device which is reflected in the drifting curves in time in Fig. 2(b). Both σ's, roughly speaking, ranges from 0.1 nA to 1.5 nA depending on regions, slope or plateau, which are large numbers considering the current magnitude is order of 10 nA. Because of the instability of the device, the original purpose for the assessment of the uncertainty of the KNN algorithm appears to be partially fulfilled. However, the most promising result is that its intrinsic uncertainty must be much less than σ^{m} and σ^{KNN}. The stability of the KNN algorithm is well reflected in the match of the data points (red solid circles) of $I^{\mathrm{m,KNN}}$ with I^{KNN} curve in Fig. 2(b). Here, $I^{m,\mathrm{KNN}}$ represents the measurements performed by the KNN regression process in KNN algorithm. Figure 2(b) shows drifting curves which are well discerned by the dates of the data acquisition time.

For the control of the measurement instruments, such as voltage sources and current multimeter the PyVISA package was utilized. The PyVISA package is a Python package that facilitates the control of any measurement device, irrespective of its interface (e.g. GPIB, RS232, USB, Ethernet)[5].

For further investigation, we are going to apply our programs to the assessment of the pumping error of our single electron pumps as well as the uncertainty evaluations.

III. STATISTICAL ANALYSIS

$I_i^{\mathrm{m}}(x, y)$ is the current measured at gate voltages of x and y where m and i stands for measurement and index of the 3D array, respectively. $I_i^{\mathrm{p}}(x, y)$ is the current predicted by the KNN algorithm at gate voltages of x and y where p, i stands for the prediction and index of the 3D array, respectively. The arrays of $I_i^{\mathrm{m}}(x, y)$ and $I_i^{\mathrm{p}}(x, y)$ are (20, 200, 200) where 20 and represents the number of each corresponding experiments (N_{exp}).

$$\sigma^{\mathrm{m(KNN)}}(x,y) \equiv \sqrt{\sum_{i=1}^{N_{\mathrm{exp}}} (I_i^{\mathrm{m(KNN)}}(x,y) - \langle I_i^{\mathrm{m(KNN)}}(x,y)\rangle)^2 / N_{\mathrm{exp}}} \tag{1}$$

$$\langle I_i^{\mathrm{m(KNN)}}(x,y)\rangle = \sum_{i=1}^{N_{\mathrm{exp}}} I_i^{\mathrm{m(KNN)}}(x,y)/N_{\mathrm{exp}} \tag{2}$$

$$\tag{3}$$

IV. DETAILS OF KNN MEASUREMENT

~~I^{m} is measured current by sweeping x for each fixed y which is iterated for varied y, for instance x starts sweeping from 0 to -1 V and y is varied in step-wise from 0.3 to 0.5 V. Thus, x and y are digitized points of 200×200. Once sweeping x is ended, the next sweep starts again from the same point, for instance 0 V, but with varied y value. The time taken for moving from one to another point is set to 0.2 s. Eventually it takes about 7 hrs to scan the 200×200 points. $I^{\mathrm{m,\ KNN}}$ is KNN regression algorithm-assisted measured current while I^{KNN} is predicted value from the KNN regression algorithm by fitting the KNN parameters to $I^{\mathrm{m,\ KNN}}$. Our program is designed to start training process from 36 points of $I^{\mathrm{m,\ KNN}}$. The number of $I^{\mathrm{m,\ KNN}}$ is increased one by one when the variance of the predicted I^{KNN} is beyond the criteria, for instance the criteria parameter tolsig is set to 0.001. Six different models of KNN are used to calculate the variance. (x, y) scan jumps from one point to another by the programmed distance. 0.3 s (time.sleep) is set to be a waiting time for the system to stabilize after the jumping. One of the advantages of KNN -assisted measurement is the time savings. The number of $I^{\mathrm{m,\ KNN}}$ points is roughly 33 % of the total number of I^{KNN} points. However, the real measurements took about 7 times that of I^{KNN}. The longer time taken for I^{m} is due to the time taken for returning the sweep process to the start point.~~

I^{m} is measured by sweeping x for each fixed y, which is iterated for varied y. For instance, x sweeps from 0 to -1 V and y varies in steps from 0.3 to 0.5 V. Thus, x and y are digitised points of 200×200. It is important to note that once the x-sweep is complete, the subsequent sweep resumes from the same point, for example, 0 V, but with a varied y value. The time allocated for transitioning between these points is set to 0.2 s. The total time required to scan the 200×200 points is approximately 7 hours. $I^{\mathrm{m,\,KNN}}$ is defined as the KNN regression algorithm-assisted measured current, while I^{KNN} is the predicted value from the KNN regression algorithm by fitting the KNN parameters to $I^{\mathrm{m,\,KNN}}$. The program is designed to initiate the training process from 36 points of $I^{\mathrm{m,\,KNN}}$. The number of $I^{\mathrm{m,\,KNN}}$ is increased incrementally when the variance of the predicted I^{KNN} exceeds the predetermined criteria, for instance, the criteria parameter 'tolsig' is set to 0.001. Six distinct KNN models are employed to calculate the variance. (x, y) scan traverses from one point to another at a programmed distance. The system is set to a waiting time of 0.3 s (time.sleep) after the jump to allow for system stabilisation. A key benefit of KNN-assisted measurement is the significant reduction in time. The number of I^{m} points is approximately 33% of the total number of I^{KNN} points, yet the actual measurements of I^{m} are approximately seven times those of I^{KNN}. The longer time taken for I^{m} is due to the time taken for returning the sweep process to the start point.

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[3] https://www.bipm.org/en/si-base-units/ampere; The ampere, symbol A, is the SI unit of electric current. It is defined by taking the fixed numerical value of the elementary charge e to be

$1.602176634 \times 10^{19}$ when expressed in the unit C, which is equal to A s, where the second is defined in terms of $\Delta\nu_{Cs}$.

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[5] https://pyvisa.readthedocs.io/en/latest/

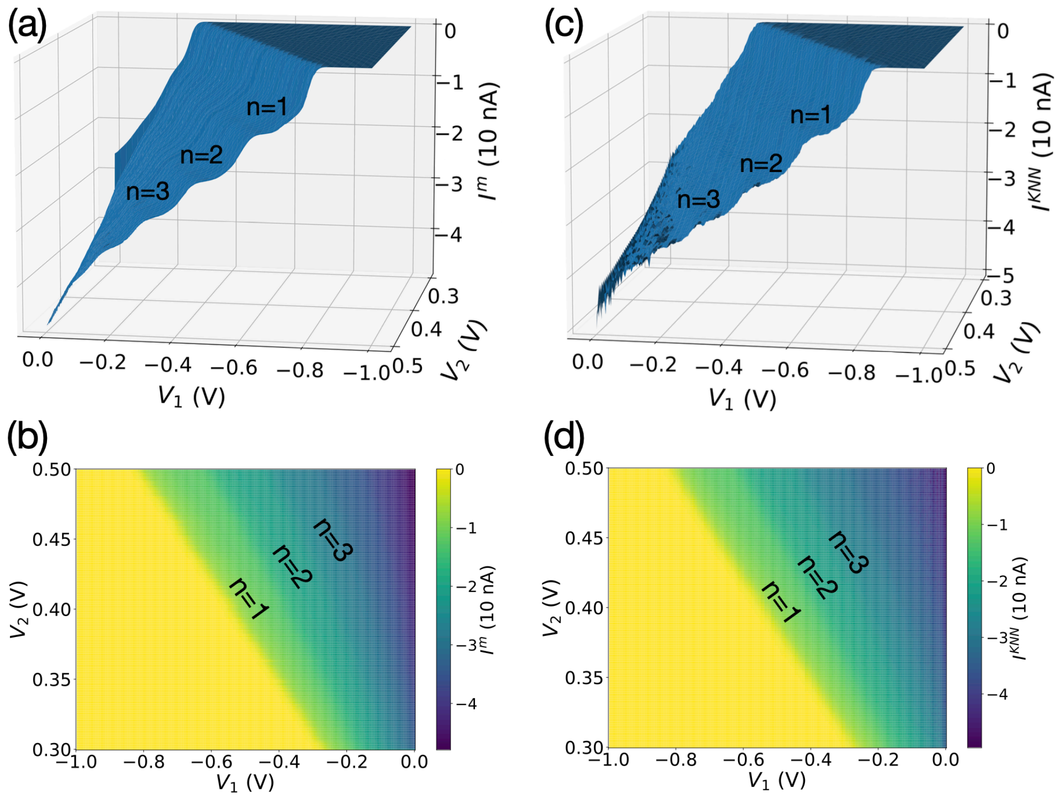

Fig. 1: 3D surface plot (a) and heat map (b) of currents measured I^{m} through a QPC whose number of electron-transport channel is quantized as n where n is an integer number. (c) and (d) corresponds to KNN program-created 3D surface plot and heat map (I^{KNN}), respectively. The number of data points are 200 by 200. The time taken to achieve the data is about 7 hours for (a) and 1 hour for (c).

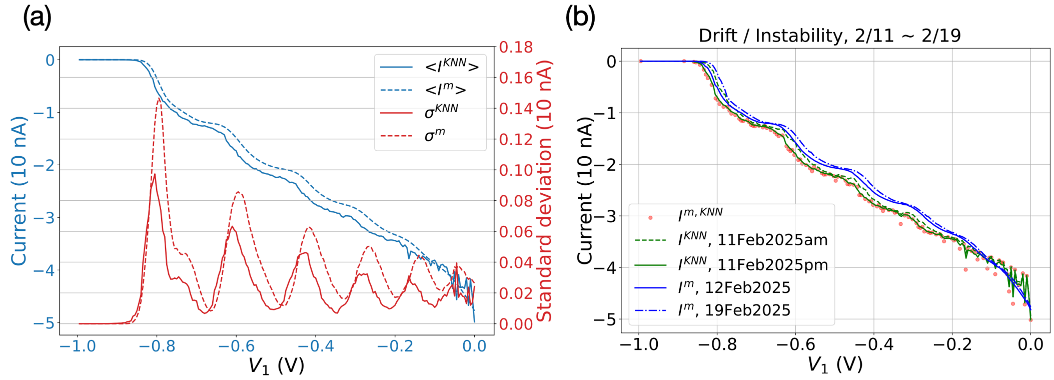

Fig. 2: (a) Comparison of currents measured (I^{m}) and obtained (I^{KNN}) by KNN algorithm with their standard deviations σ^m and σ^{KNN}, respectively. For the statistical analysis 14 and 20 set of experiments (N_{exp}) have been performed to obtain σ^m and σ^{KNN}, respectively with each experiment consists of 200×200 data points. (b) $I^{m,\mathrm{KNN}}$ represents the measurements performed by the KNN regression process in KNN algorithm. The five data curves were obtained one after another during 8 days. $V_2 = 0.5$ V.